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Research Article

Theoretical Analysis and Simulation of SiO_2 and ZrO_2 Based Antireflective Coatings to Improve Crystalline Silicon Solar Cell Efficiency

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ABSTRACT

The Solar cell efficiency is crucial, and optical losses can hinder it significantly. Anti-reflective coatings are effective in minimizing these losses. In our study, we used Fresnel equations to calculate reflectance values for single-layer SiO_2, ZrO_2, a SiO_2-ZrO_2 mixture, and a double-layer SiO_2/ZrO_2 configuration. We then assessed their impact on crystalline silicon solar cells using the SCAPS program. The reflectance values of single-layer SiO_2, ZrO_2 and 10%SiO_2-90%ZrO_2 mixture were calculated as 19.17%, 13.09% and 13.01%, respectively. Notably, the double-layer SiO_2/ZrO_2 coating showed a low reflectance of 7.58%, a significant improvement compared to uncoated silicon at 37.45%. Efficiency values for crystalline silicon solar cells were calculated for single layer as 18,95% (SiO_2), 20.39% (ZrO_2), 20,40% (mixed coating) respectively and 21.68% for the double-layer SiO_2/ZrO_2 configuration.

1. Introduction

Zirconium dioxide (ZrO_2) thin films are widely used in science, technology and industry, with various applications such as optical filters, photocatalysts, and transistors [1-3]. ZrO_2 is found in three different phases: monoclinic (1443K), tetragonal (1443-2643K) and cubic (2643-2953K) at different annealing temperatures and has a stable structure in these temperature ranges [4]. When the cubic phase of the ZrO_2 thin films is considered, it has a band gap of 6.1 eV and a refractive index of around 2 [5, 6]. Because of these properties of ZrO_2 thin films can be used as an anti-reflective coating for crystalline silicon solar cells. Anti-reflective coatings can be applied to the top surface of crystalline silicon solar cells as one or more layers of thin films. The minimum reflection condition of anti-reflective thin films is related to the thickness and refractive index of the thin films.
These conditions can be expressed as [7],

$$n_1 = \sqrt{n_0 n_2} \quad (1)$$

$$d_1 = \frac{\lambda_0}{4\eta_1} \quad (2)$$

ZrO_2 thin films can be easily produced by methods such as vacuum evaporation, sputtering, pulsed laser deposition, ion-assisted deposition, ion beam sputtering, and Sol-gel [8-10]. However, it is important both in terms of time and cost to calculate the film thickness for the appropriate reflectance value of the film to be coated and to carry out the experiments in this direction. Therefore, the thickness value of the materials to be coated can be easily calculated with Fresnel equations to obtain the ideal reflectance value of the single-layer and double-layer films. While some of the sun rays coming to the surface of the solar cell are reflected back from the surface, some of them may pass through the surface and cause current formation in the solar cell. By using anti-reflective coatings, light reflection can be reduced, and transmittance can be increased. In this way, higher efficiency solar cells can be produced. The Fresnel equations in which the reflection value is measured for anti-

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reflective coatings are given in eq (3) and eq (4) for single layer and double layer, respectively.

$$R_{SL} = |r^2| = \frac{r_1^2+r_2^2+2r_1r_2\cos2\theta}{1+r_1^2r_2^2+2r_1r_2\cos2\theta} \quad (3)$$

where; $r_1 = \frac{n_0-n_1}{n_0+n_1}$, $r_2 = \frac{n_1-n_2}{n_1+n_2}$, $\theta = \frac{2\pi n_1 d_1}{\lambda}$

$$R_{DL} = \frac{A+B+C+D+E+F}{1+(r_1^2r_2^2)+(r_1^2r_3^2)+(r_2^2r_3^2)+C+D+E+F} \quad (4)$$

where;

$r_1 = \frac{n_0-n_1}{n_0+n_1}$, $r_2 = \frac{n_1-n_2}{n_1+n_2}$, $r_3 = \frac{n_2-n_3}{n_2+n_3}$,

$\theta_1 = \frac{2\pi n_1 t_1}{\lambda}$, $\theta_2 = \frac{2\pi n_2 t_2}{\lambda}$ and

A = $r_1^2+r_2^2+r_3^2$, B= $r_1^2r_2^2r_3^2$,

C = $2r_1r_2(1+r_3^2)\cos2\theta_1$,

D = $2r_2r_3(1+r_1^2)\cos2\theta_2$,

E = $2r_1r_3\cos2(\theta_1+\theta_2)$,

F = $2r_1r_2^2r_3\cos2(\theta_1-\theta_2)$

In this study, reflectance calculations were made for the first layer of anti-reflective layer ZrO_2 thin film and for the second layer, SiO_2 thin films with good optical transmittance and passivation effect in solar cells [11], and average reflectance values were obtained. In order to investigate the anti-reflective effect of SiO_2 and ZrO_2 mixtures, the refractive index of the mixture at various ratios was calculated with the Arago-Biot (A-B) equation and the reflectance values were calculated. In addition, the different equations for calculating the refractive index of mixtures are expressed as;

Arago-Biot (A-B) : $n=n_1\phi_1+n_2\phi_2$ (5)

n=Refractive index of mixture, n_1=Refractive index of pure component-1, n_2=Refractive index of pure component-2, ϕ_1=Volume fraction of pure component-1 and ϕ_2=Volume fraction of pure component-2 Where, also $\phi_1=x_1V_1/\Sigma x_iV_i$ and $\phi_2=x_2V_2/\Sigma x_iV_i$ here x is the mole fraction V_i is the molar volume of component i [12-14].

2. Methodology and Simulation

In our research, we conducted an analysis of the average reflectivity values for single-layer Zirconium Dioxide (ZrO_2), Silicon Dioxide (SiO_2), and double-layer SiO_2/ZrO_2 thin films, as well as the average reflectivity values of SiO_2-ZrO_2 mixtures at varying ratios. These calculations were performed using eq (3) and eq (4). Furthermore, we determined the refractive indices of SiO_2-ZrO_2 mixtures with different composition ratios employing the Arago-Biot (A-B) formula presented in eq (5). Additionally, to explore the impact of average reflectivity values on crystalline silicon solar cell parameters, we employed the numerical simulation program SCAPS.

SCAPS is a versatile software tool capable of simulating various thin-film solar cell types, including solar cells, Copper Indium Gallium Selenide (CIGS) cells, Cadmium Telluride (CdTe) cells, Gallium Arsenide (GaAs) cells, crystalline silicon (c-Si) cells, and amorphous Silicon (a-Si:H) cells, as described in references [15, 16]. The SCAPS program performs calculations involving steady-state band diagrams, recombination profiles, and carrier transport in one dimension, based on Poisson's equation and the continuity equations for both holes and electrons [17].

3. Result and Discussion

This study was conducted in three sequential stages. In the initial stage, we computed the reflectance values of single-layer ZrO_2, SiO_2, and double-layer SiO_2/ZrO_2 thin films using Fresnel equations. Subsequently, in the second stage, we determined the refractive indices of SiO_2, ZrO_2, mixtures across various ratios and calculated reflectance values dependent on fim thickness.
Finally, in the third stage, we applied the average reflectance values of single-layer SiO_2, ZrO_2, SiO_2-ZrO_2 mixtures, and double-layer SiO_2/ZrO_2 thin films as anti-reflective coatings to crystalline silicon (c-Si) solar cells using the SCAPS solar cell program. To calculate the reflectance values of SiO_2 and ZrO_2 thin films at different thicknesses, we systematically varied the thicknesses from 30nm to 100nm and summarized the obtained reflectance values in Figure 1.

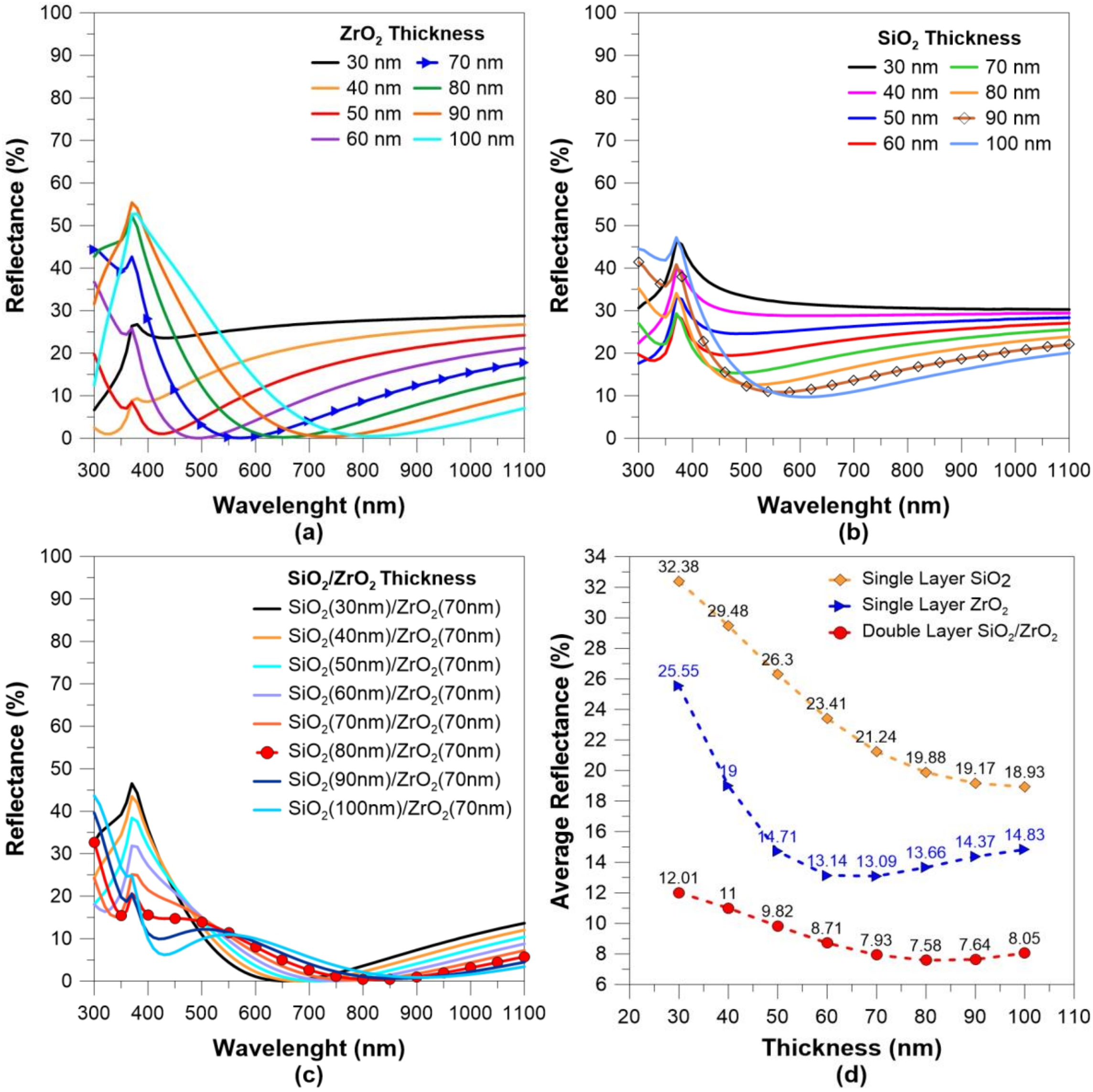

Figure 1. Reflective values of single-layer ZrO_2 (a) single-layer SiO_2 (b), double layer SiO_2/ZrO_2 (c) and average reflectance values (d)

As depicted in Figure 1(a), for ZrO_2 thin films with low thicknesses, high reflectance values were observed. With increasing thickness, both the reflectance values significantly decreased, and the minimum reflectance point shifted towards longer wavelengths. Figure 1(d) illustrates that the lowest average reflectance value for ZrO_2 thin films, 13.09%, was achieved at a thickness of 70nm. Additionally, as the thickness of the single-layer SiO_2 thin film increased, the average reflectance values decreased, reaching a minimum of 19.17% for a thickness of 90nm.

By employing multiple anti-reflective layers in solar cells, the reflective properties can be further reduced, thereby enhancing solar cell efficiency [18]. The reflectance values of double-layer anti-reflective coatings can be readily calculated using Eq (4). The thickness of the ZrO_2 thin film, previously determined as the optimal thickness, was held constant at 70nm, while the thickness of the SiO_2 thin film was varied between 30nm and 100nm. in order to achieve the lowest reflectance value. The reflectivity of the SiO_2/ZrO_2 double-layer thin film decreased from 12.01% to its lowest point of 7.58% when the SiO_2 thin film reached a thickness of 80nm. When the thickness of the SiO_2 thin film was increased from 80nm to 100nm, the average reflectivity value increased from 7.58% to 8.05%. In the literature, it is commonly observed that double-layer thin films offer advantages in terms of anti-reflective properties, leading to lower levels of reflection compared to single-layer thin films [19, 20]. When two materials with different refractive indices are mixed at different rates, the refractive index of the mixture is expected to be a value between the refractive indices of both materials included in the mixture ($n_{Low}<n_{Mix}<n_{High}$).

Based on the refractive indices of SiO_2 and ZrO_2 materials, the refractive indices of SiO_2-ZrO_2 mixtures at different ratios were calculated using eq (5) at nine different ratios

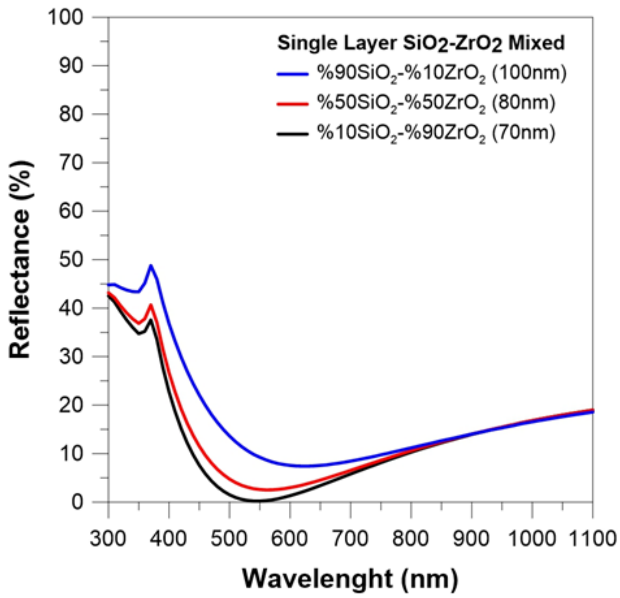

Figure 2. Graph of the reflectance of three different ratios of SiO_2-ZrO_2 mixed

Table 1. Refractive index of SiO_2-ZrO_2 mixtures at different ratios and reflectance values depending on different thickness values

		Average Reflectance (%)							
Mixed Ratio	**n(mixed)**	**30nm**	**40nm**	**50nm**	**60nm**	**70nm**	**80nm**	**90nm**	**100nm**
%90SiO$_2$-%10ZrO$_2$	1.49	31.79	28.47	24.91	21.81	19.62	18.36	17.78	17.66
%80SiO$_2$-%20ZrO$_2$	1.55	31.19	27.45	23.53	20.29	18.16	17.03	16.61	16.62
%70SiO$_2$-%30ZrO$_2$	1.60	30.58	26.42	22.19	18.88	16.87	15.92	15.65	15.80
%60SiO$_2$-%40ZrO$_2$	1.66	29.96	25.40	20.91	17.61	15.76	15.01	14.91	15.17
%50SiO$_2$-%50ZrO$_2$	1.71	29.33	24.38	19.69	16.48	14.85	14.30	14.36	14.73
%40SiO$_2$-%60ZrO$_2$	1.77	28.70	23.38	18.57	15.51	14.12	13.78	13.99	14.46
%30SiO$_2$-%70ZrO$_2$	1.82	28.06	22.41	17.55	14.71	13,58	13.44	13.80	14.33
%20SiO$_2$-%80ZrO$_2$	1.88	27.43	21.48	16.65	14.07	13.21	13.27	13.75	14.31
%10SiO$_2$-%90ZrO$_2$	1.93	26.81	20.61	15.88	13.61	13.01	13.26	13.84	14.40

Considering the refractive index of SiO_2 as 1.44 [21] and of ZrO_2 as 2.05 [22], it is clearly seen from table 1 that the refractive index of SiO_2-ZrO_2 mixture varies between 1.49 and 1.93. Eq (5) was used for the refractive index of each SiO_2-ZrO_2 ratios, and the reflectance values were calculated with the eq (3) by changing the thin film thicknesses from 30nm to 100nm. Calculations were made by taking molarity of SiO_2 and ZrO_2 as equal. It was seen that the mole fractions of SiO_2 and ZrO_2 changed in direct proportion to $V_{SiO2}/(V_{SiO2}+V_{ZrO2})$ and $V_{ZrO2}/(V_{SiO2}+V_{ZrO2})$, respectively.

The reflection-wavelength graph for three different ratios (10%SiO_2-90%ZrO_2, 50%SiO_2-50%ZrO_2, 90%SiO_2-10%ZrO_2) is given in figure 2. It can be clearly seen from table 1 that the lowest average reflectance value of 10%SiO_2-90%ZrO_2 mixture was calculated as 13.01% for the 70nm thickness. It was also noted that as the SiO_2 ratio in the mixture increased, the refractive index of the mixture decreased and therefore the average reflectance values decreased. In addition, as the SiO_2 ratio increases, the thin film thickness required to be coated in order to obtain low reflectance values also increases.

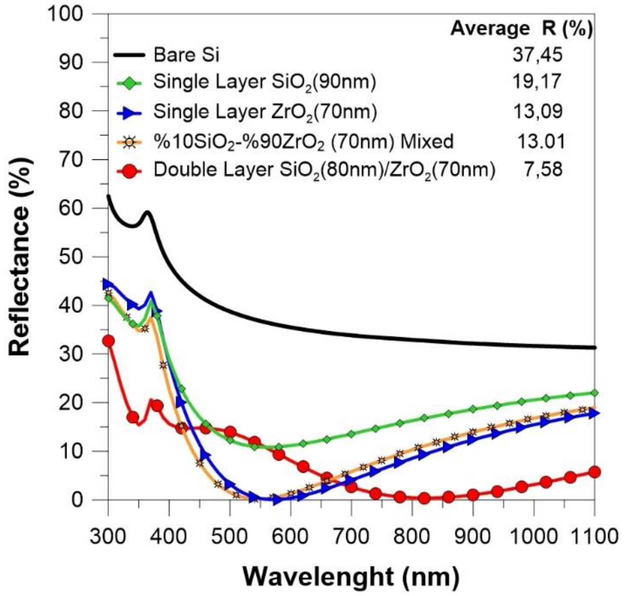

Figure 3. Reflection-wavelength graphs of different thin films

When the refractive indices of SiO_2-ZrO_2 mixtures at different ratios were examined, it was seen that the average reflectance value decreased as the refractive index approached 2. Unfortunately, the desired reflection values cannot be achieved even if ideal refractive index materials are produced for anti-reflective coatings with the mixture of two different materials in different ratios. From the reflectance wavelength graphs given in figure 3, it is clearly seen that the reflectance values of double layer SiO_2/ZrO_2 thin films give better results compared to the single layer reflectance values. While the best reflectance value in single layer layers was 13.01% for 10%SiO_2-90%ZrO_2 thin film, this value decreased to 7.58% for double layer SiO_2/ZrO_2 thin film. Therefore, multi-layer anti-reflective coatings are highly preferred for high-efficiency solar cells due to their low reflectance values [23].

The average reflectance values of single layer SiO_2, single layer ZrO_2, single layer %10SiO_2-%90ZrO_2 mixed and double layer SiO_2(80nm)/ZrO_2(70nm) thin films and the initial parameters of the crystalline silicon solar cell given in table 2 were used together in the SCAPS program to investigate the effect of anti-reflective coatings on the crystalline silicon solar cell. Figure 4 shows a schematic representation of conventional crystalline silicon solar cells.

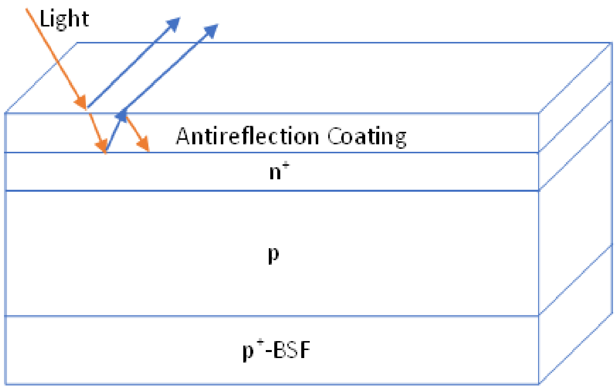

Figure 4. Schematic representation of Crystalline silicon solar cell

The current-voltage graph of this solar cell is given in figure 5 and the parameters of the solar cell are summarized in table 3. As can be seen from table 3, anti-reflective coatings have a great effect on solar cell parameters. For the uncoated c-Si solar cell, the V_{oc}, J_{cs}, FF and efficiency values were calculated as 752.20V, 25.48mA/cm^2, 82.80% and 14.63%, respectively, and serious improvements were achieved on the solar cell parameters by applying anti-reflective coating to the solar cells. For example, the efficiency values for single layer SiO_2 increased from 14.63% to 18.95% compared to the uncoated solar cell. In addition, the efficiency values for single layer ZrO_2, single layer 10%SiO_2-90%ZrO_2 mixed and double layer SiO_2-ZrO_2 were recorded as 20.39%, 20.40% and 21.68%, respectively

Table 2. Some initially parameters of c-Si solar cell for SCAPS [24]

	n^+	p-Si	p^+-Si-Bsf
Thickness (µm)	0.3	200	7
Bandgap (eV)	1.12	1.12	1.12
Electron affinity (eV)	4.05	4.05	4.05
Dielectric permittivity	11.90	11.90	11.90
CB effective density of states (cm^{-3})	4.79x10^{18}	2.80x10^{19}	2.80x10^{19}
VB effective density of states (cm^{-3})	4.52x10^{18}	1.04x10^{19}	1.04x10^{19}
Electron mobility (cm^2/Vs)	73.36	1041	202
Hole mobility (cm^2/Vs)	155.6	412	77
Shallow uniform donor density N_D (cm^{-3})	1x10^{20}	1x10^{16}	-
Shallow uniform acceptor density N_A (cm^{-3})	-	1x10^{16}	1x10^{19}

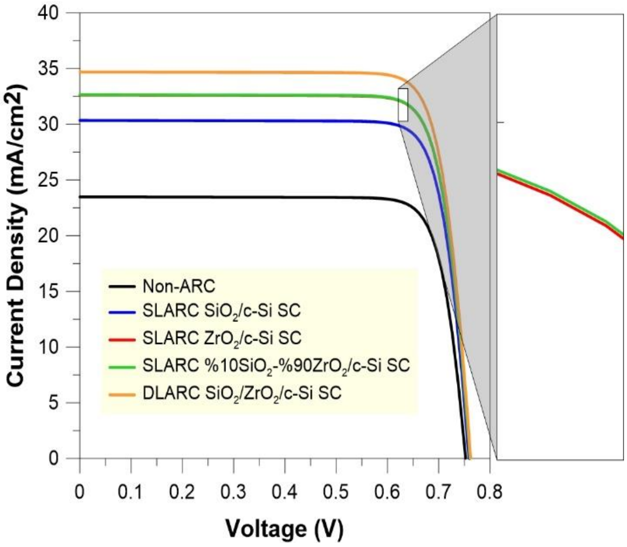

Figure 5. I-V graphics of crystalline silicon solar cell of uncoated and different anti-reflective coating

Table 3. The effect of different anti-reflective coatings on crystalline silicon solar cells

	V_{oc}(mV)	J_{sc}(mA/cm^2)	FF(%)	Eff.(%)
Non-ARC/c-Si SC	752.2	23.48	82.80	14.63
SLARC SiO_2/c-Si SC	758.9	30.34	82.30	18.95
SLARC ZrO_2 /c-Si SC	760.8	32.62	82.12	20.39
SLARC %10SiO_2/%90ZrO_2 Mixed/c-Si SC	760.8	32.66	82.12	20.40
DLARC SiO_2/ZrO_2/c-Si SC	762.4	34.69	81.95	21.68

4. Conclusions

This study investigated the potential of anti-reflective coatings, specifically single-layer SiO_2, ZrO_2, SiO_2-ZrO_2 mixtures, and double-layer SiO_2/ZrO_2 thin films, to enhance the performance of crystalline silicon solar cells. Reflectance calculations and refractive index assessments were conducted for various coating configurations, and their impact on solar cell efficiency was investigated using the SCAPS program. The results demonstrated significant improvements in solar cell parameters with the application of anti-reflective coatings. Single-layer SiO_2, ZrO_2, and SiO_2-ZrO_2 mixtures all showed enhanced efficiency compared to uncoated solar cells. Furthermore, the double-layer SiO_2/ZrO_2 configuration exhibited the highest efficiency among the coatings studied.

These findings emphasize the critical role of anti-reflective coatings in increasing the efficiency of crystalline silicon solar cells, paving the way for more efficient and sustainable solar energy conversion technologies. The utilization of multi-layer anti-reflective coatings, such as double-layer SiO_2/ZrO_2, is particularly promising for achieving low reflectance values and maximizing solar cell performance.

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The Declaration of Conflict of Interest/ Common Interest

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