

Optical Effect of Pure and Metal Doped SLARC on Silicon Solar Cell

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Abstract

The reflection losses of the silicon solar cells are significant, and minimization of such losses can be facilitated by antireflection coatings (ARC). In this work, theoretical investigation on the optical properties of ZrO_2 and HfO_2 thin films working as ARC is carried out. Further, the permittivities of these ZrO_2 and HfO_2 is manipulated by doping with metals like Ag, Ni and Co. Optimization of the filling fraction of the metals in the HfO_2 and ZrO_2 improved the stability and durability of these thin film ARCs as well as reduces the optical losses to a greater extent. By the application of the ARCs, the absorbed photon flux increases and hence improvement in the efficiency of the solar cell is observed.

Keywords: Photovoltaic conversion, Anti reflecting coating, silicon solar cell and photovoltaic

Introduction

Photovoltaic (PV) transformation of sun powered vitality starts to form a important commitment to control era in numerous locales, with more than 90% of the around the world PV industry depending on sun based cells based on silicon semiconductors. Wafer-based silicon solar cells account for the majority (over 90%) of the global PV market. This is largely because silicon (Si) has a bandgap that is suitable for efficient PV conversion, it is the second-most abundant material in the earth's crust, it is nontoxic, and the chemical and semiconductor industries are well-versed in its technology. The PERL cell based on p-type silicon [1] set a new record for energy conversion efficiency of silicon solar cells in the lab in 1999, reaching a new high of 25%. This record stood for the following 15 years [2]. The record efficiency increased to 25.6% in 2014 and to 26.7% in 2017 [3] owing to the heterojunction (HJ) intrinsic thin layer technology based on Si passivating layers and interdigitated back contacts (IBCs) on n-type silicon wafers. Wafer-based silicon modules have an efficiency of 24.4% and are advancing both in the lab and commercially [4, 5]. The best method to measure the power of silicon technology is to look at the international technology roadmap for photovoltaics [6].

However, one of the drawbacks of silicon solar cell is that its electronic bandgap is narrow, making it a poor absorber of long wavelength light. A somewhat thick (100 nm - 500 m) silicon structure has traditionally been used to offset this [7]. Larger silicon does boost solar absorption, but it also raises material costs for large-area applications and stiffens the structure. In addition, non-radiative recombination of photogenerated charge carriers causes inevitable losses in power conversion efficiency in thick silicon solar cells [8] along their rather long trip to electrical contacts at the cell's extremities. In order to effectively collect the photoexcited electron-hole (e-/h+) pairs with minimal to no losses, a solar cell must be both optically thick (able to absorb all or most of the incident sunlight) and electrically thin. These two conditions result in the best thickness for maximum efficiency. As a result, we must address both the optical and electrical issues to comprehend the limiting efficiency. The short-circuit current density of a solar cell is dependent on the density of photogenerated carriers. The system's reflectance phenomenon causes the largest

number of photogenerated carriers to be lost or reflected outwards, reducing efficiency. The incoming light radiation loss must be minimized by decreasing the solar cell surface reflection to construct high efficiency solar cells [9].

Choosing the proper thin film antireflection coating (ARC) layer for high-efficiency solar cells is crucial. The quantity of incident photons reaching the active portions of the solar cell must be maximised, the short-circuit current (J_{sc}) must be enhanced, and an adequate thin film ARC must be used to reduce reflection losses. A variety of high refractive-index ARC materials such as ZrO₂, HfO₂, TiO₂, Al₂O₃, Si₃N₄, Ta₂O₃, MgF₂, and SiO₂ have so far applied in the fabrication of Si solar cells [10]. Recently Lin *et al.*, reported SiO₂/TiO₂ composite ARC on solar cells, demonstrated excellent refractive index and transparency, and have been effectively coated as using the PECVD method, yet with a reflectance of 10% [11]. Mechanical characteristics are also important to examine when choosing an ARC coating material. The selection of a high index material varies on the application but is frequently a trade-off between optical qualities, cost, and durability. For ARC applications, durability is a crucial consideration. Use Hafnium dioxide (HfO2) instead as a result, as it has excellent scratch resistance, is inexpensive, abundant, and self-cleaning. [12].

HfO₂ has been the subject of much research because of its exceptional electrical, optical, photocatalytic, biological, and mechanical properties. HfO₂ has a broad-spectrum gap in the visible range, a high threshold for induced laser damage, strong thermal conductivity, low transparency, and excellent transmittance, to name just a few of its optical and electrical properties. The metal doped dielectric layers served as a multifunctional layer that included antireflective and self-cleaning properties [12]. The most effective metal doped dielectric ARCs were used to improve physical properties such robustness, high corrosion resistance, scratch resistance, and great surface roughness. To improve the mechanical characteristics of HfO₂ based coatings, a technique including doping the coatings with metals like silver, nickel, or cobalt has been developed. As compared to bare ZrO₂ and HfO₂, the suggested Ag/Ni/Co doped HfO₂ have significantly enhanced the physical, mechanical, and electrical characteristics of ZrO₂ and HfO₂ [13]. ZrO₂ and HfO₂ reduce reflectance while simultaneously enhancing optical transmittance in the visible and near-infrared spectrum when photons from the sun's spectrum are injected into the device. This enhances the device's electrical conductivity [13, 14]. The highest power conversion efficiency,

according to Shah et al., was attained by the fabricated Si solar cell with double ZnO/Ag-doped ZnO AR layer, which was 9.48%. The lowest efficiencies were attained by the fabricated crystalline Si solar cells with single ZnO ARC and single Ag-doped ZnO AR layers, which were, respectively, 8.59% and 8.78%. This work explores the anti- reflection properties of bare HfO₂ and Ag, Ni and Co doped HfO₂ on Si substrate and the influence of optical transmittance on electrical properties on Si solar cell. The filling percentage of metals in HfO₂ was adjusted as a result of this study, which boosted the transmittance and durability of these thin film ARCs while decreasing optical losses. The absorbed photon flux rises resulting in a 2.5 - 5% increase cell efficiency.

2. Numerical calculation

2.1 Optical properties of bare and ARC coated Si substrate

The Fresnel reflection coefficient from bare silicon for light incident from air is given by [16].

The Reflectance of single ARC on solar cell;

$$R = \left| r \right|^2 = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos 2\theta}{1 + r_1^2r_2^2 + 2r_1r_2\cos 2\theta}$$
(2)

 $r_1 = \frac{n_0 - n_1}{n_0 - n_1}, r_2 = \frac{n_1 - n_2}{n_1 - n_2}, \theta = \frac{2\pi nt}{\lambda}, t \text{(thickness)} = \frac{\lambda_0}{4n} \text{ (center wavelength } (\lambda_0)\text{)}$

where n_0, n_1 and n_2 are refractive indices of air ARC (HfO₂/ZrO₂) and Si



Fig. 1. HfO₂ ARC on Si Substrate

2.2. Effective refractive index of metal doped HfO₂

Permittivity of metals are calculated from [16]

$$\varepsilon_r = \varepsilon_r + i\tilde{\varepsilon}_r = (n + ik)^2$$
(3)

$$\varepsilon_r = n^2 - k^2$$

$$\tilde{\varepsilon}_r = 2nk$$

2.3. Effective permittivity and refractive index of metal doped HfO_2

The effective permittivities of the Ag/Ni/Co doped HfO₂ ARC can be estimated first using the Maxwell-Garnett effective medium theory (EMT). [9, 17]. For the permittivity components parallel and perpendicular to the over layers obtain

$$\varepsilon_{\Box} = \rho \varepsilon_{m} + (1 - \rho) \varepsilon_{d} \qquad (4)$$
$$\varepsilon_{\bot} = \frac{\rho}{\varepsilon_{m}} + \frac{(1 - \rho)}{\varepsilon_{d}} \qquad (5)$$

The subscripts in this instance, and, denote permittivity elements for electric field orientations parallel and perpendicular to the plane of layers, respectively. where m and d are the relative permittivities of the constituent metal and dielectric substances, and is the volumetric percentage of the constituent metal layers [18]. The filling fraction of the metal

$$\rho = \frac{t_m}{t_m + t_d} \tag{6}$$

The effective permittivity of Ag/Ni/Co doped HfO2

$$\varepsilon_{eff} = \begin{bmatrix} \varepsilon_{\Box} & 0 & 0\\ 0 & \varepsilon_{\Box} & 0\\ 0 & 0 & \varepsilon_{\bot} \end{bmatrix}$$
(7)



Fig. 3. Metal doped ARC on Si substrate

The effective refractive index of Ag/Ni/Co doped HfO2

Effective refractive index (n) = $\sqrt{\mathcal{E}_{eff}}$

2.4. Absorbed Photon flux of Si solar cell

Absorbed photon flux is
$$A = \phi_0(1-R) - \phi(d)$$
 (9)

where $\phi_0(\lambda) = P(\lambda) \times \frac{\lambda}{hc}$ (Photon flux of various wavelength range (400 nm -1000 nm))

and corresponding to the irradiance of $P=1000 \text{Wm}^{-2}$

$$\phi(d) = \phi_0 (1 - (R) - \exp[-\alpha(\lambda) * d]$$
 (10)

where $\alpha = 2.303 \times \frac{A}{d}$, d = 30 nm

2.5. Electrical properties

The related Jsc values are determined by incorporating the solar AM1.5G spectrum, where e denotes the electronic charge, denotes the incident wavelength, h denotes the Planck's constant, c denotes the speed of light, $I(\lambda)$ denotes the solar AM1.5G spectral density, and A (λ) denotes the absorption coefficient, which can be measured or calculated as A (λ) = 1-R (λ). The short circuit current is

$$J_{sc} = \frac{e}{hc} \int_{400}^{900} I(\lambda) A(\lambda) \lambda \,\mathrm{d}\,\lambda \qquad (11)$$

The Open circuit voltage

$$V_{OC} = \frac{KT}{e} \ln(\frac{J_{sc}}{J_0} + 1) \quad (12)$$

 J_{ph} calculated from equation (11)

The fill factor is calculated [31] using the equation

$$FF = \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc} + 1}$$
(13)
where $v_{oc} = \frac{eV_{oc}}{kT}$ is a normalised voltage

$$I_{sc} = -I_{ph} \tag{14}$$

$$I = -I_{ph} + I_d \tag{15}$$

$$I_{d} = -I_{ph} \left[\exp(\frac{eV}{K_{B}T}) - 1 \right] \quad (16)$$

$$\eta = \frac{J_{ph} * V_{oc} * FF}{P_{in}} \tag{17}$$

3. Result and discussion:

3.1Reflectance analysis of HfO2 on Si Substrate

Equation (1) is used to calculate the reflectance of the single layer of ARC HfO_2 on Si of the silicon solar cell. As can be seen in fig. 3(a), Green et al.'s [2] calculation of the Si substrate's reflectance revealed that it exceeded 55%. Calculating the reflection of the single ARC layer of HfO_2 uses the refractive index data from [2]. The reflectance of the Si substrate with the HfO_2

single layer ARC is comparable and less than 30% across the visible wavelength range, and zero reflectance is attained at 400-600 nm, as illustrated in fig. 3(b) [19].



Figure 3(a) Reflectance of Silicon substrate 3(b) Reflectance of

3.2 Analysis of effective refractive index of metal doped HfO2 ARC

The Maxwell – Garnett effective medium theory, which is provided in equations (4) to (6), may be used to compute the effective permittivity of metal doped HfO₂ (7). The fill fraction is affected by the thickness of the dielectric material and metal dopant, as determined by equation (6). Figure 4 depicts the fluctuation in fill fraction as a function of the metal's (25nm) and the dielectric material's (75nm) thickness.. The effective refractive index of Ag/Ni/Co doped HfO₂ with a 0.05 fill fraction was investigated in Figure 4. In the visible region, the Ag doped HfO₂ refractive index ranges from 2.5 to 1.5, whereas the Ni/Co doped HfO₂ refractive index extends from 2.5 to 0.5.



Figure 4. Effective refractive index of Ag/Ni/Co doped HfO2

3.3 Optical analysis of metal doped HfO2

Equation (2) is used to compute the reflectance of Ag-doped HfO2, Ni-doped HfO2, and Co-doped HfO2 with various fill fractions of 0.05-0.25, as illustrated in fig. 5(a), (b), and (c). The Ag - doped HfO₂ shows increasing reflectance with increasing fill fraction and shows maximum reflection for fill fraction of 0.25. Also, at 500 nm, the reflectance is zero for fill fractions of 0.05 and 0.25. The Ni - doped HfO₂ with fill fraction 0.05 shows an excellent feature of reduced reflectivity throughout the visible wavelengths. Ni doped HfO₂ films exhibit minimum reflectivity at 500 nm and decreased reflectivity in the 700–1000 nm region when the fill percentage is increased. The Co -doped HfO₂ films of fill fraction 0.05 and 0.25 show reduced reflection at the wavelength region of 400 - 600 nm, while the films with 0.15 fill fraction show greater reflection at the higher wavelengths. Thus, by fine tuning the fill fraction of the metal dopants, the zero reflection at specific wavelength range can be achieved [19].



Figure.5. the reflectance of (a) Ag/HfO₂ (b) Ni/HfO₂ and Co/HfO₂

3.4 Effect of ARC in Absorbed Photon flux

The fig. 6 shows the absorbed photon flux of bare silicon solar cell as well as the various ARC incorporated Si solar cell. It is observed that the bare silicon suffers reflection losses and hence shows minimal absorbed photon flux. Of the employed ARC layers, the Si solar cell with Ni doped HfO₂ and Co -doped HfO₂ ARC layers show significant rise in the absorbed photon flux of $3.2e^{21}$ m²s⁻¹ compared to the photon flux of $1.5e^{21}$ m²s⁻¹ of bare silicon solar cell. The absorbed photon flux of solar cell with undoped HfO₂ is slightly higher than with the metal doped HfO₂ ARC is due to the reflection occurring due to metal dopants. The metal doped ARCs possess better stability and durability than the pure HfO₂ layer hence it is preferred to opt for metal doped ARC for Si solar cell [20].



Figure.6. Absorbed Photon flux with various Pure and metal doped ARC on Si substrate

3.5 Analysis of electrical properties

The short -circuit current density as an outcome of the optical properties of the solar cell can be calculated using equation (11) for bare Si – solar cell with ARC layers. The fig. 7 reveals that the solar cell with pure HfO₂layers as ARC show slightly higher efficiency than the solar cell with metal doped ARC layers. It is due to the fact the pure HfO₂ ARC – Si solar cell shows relatively greater absorbed photon flux than the solar cell with metal - doped ARCs.

Figure 7 showed an increase in short circuit current from 24 mA to 36 mA. According to theoretical findings, pure HfO_2 and Ag/Ni/Co doped HfO_2 are the ARCs that are best suited for silicon substrate, The lifespan (e) and diffusion coefficient (De) of photoelectrons were both lengthened by the presence of HfO_2 thin sheets. The short-circuit current (J_{sc}) was increased as a result of it helping to prevent reverse electron transfer [21].





The suggested pure HfO₂ and Ag/Ni/Co doped HfO₂ single layer anti reflection coating (SLARC) layers on Si solar cells were computationally calculated and evaluated utilising current-voltage (I-V) characteristics. Equations (11) to (17) are used to determine the I-V profiles of bare and ARC coated Si substrates in Figure 8. Table I summarizes the photovoltaic characteristics of developed solar cells using SLARC layers. The developed Si solar cells with pure HfO2 and Ag/Ni/Co doped HfO2 layers have high efficiencies of 11.7%, 12.92%, 13%, and 14.5%, respectively, while the

proposed Si solar cell with Si/HfO2 SLARC has a low power conversion efficiency (η) of 9.6%. Of the metal - doped ARCs, Co -doped HfO₂ shows excellent properties of performing as the anti – reflection coating and increases the efficiency of the solar cell to 13% which is far greater than the efficiency of 9.6% of the bare silicon solar cell [22].

The Si -solar cell with the Ni - doped HfO_2 ARC is the second best of the considered ARC incorporated solar cell with the overall efficiency of 12.92%. The Ni doped thin films exhibit high hardness and low friction and wear. Addition of Ni through doping may reduce the grain size of the thin films and hence efficiency is slightly lesser than the Co doped ARC

The Si - solar cell with the Ag - doped HfO_2 ARC shows an efficiency of 11.7% which is better than the bare silicon solar cell. Though silver possess better features of highest electrical conductivity the lesser improvement is due to the higher binding energy of each spin - orbit component for the metal atoms [23].



Figure 8. I–V Characteristics of pure HfO₂ and ZrO₂ and metal doped HfO₂ARCon Si solar cells.

Integrating a pure and Ag/Ni/Co doped HfO_2 thin film layer was placed over Si layer, considerably increasing the solar cell's light conversion efficiency from 9.6% to 14.5%. These

findings suggested that HfO_2 and optimised (0.05) metal doped HfO_2 were promising candidates for upcoming solar cell devices because they functioned as an antireflective thin film, directing the maximum transmittance with high mechanically and thermal resistance while also improving solar cell efficiency in converting electricity.

Materials	Jsc (mA)	Voc (V)	ŋ(%)
Si	23.58	0.58	9.6
Si/Ag-HfO ₂	28.5	0.6	11.7
Si/Ni-HfO ₂	31.3	0.6	12.92
Si/Co-HfO ₂	31.9	0.6	13
Si/HfO ₂	35.19	0.6	14.5

Table .1.Photovoltaic parameters for fabricated Si solar cells with Various SLAR

4. Conclusion:

The architecture for creating pure and Ag/Ni/Co doped HfO₂ single ARC on Si solar cells is described in this study, along with examples of the solar cells' optical, structural, and photovoltaic characteristics. The fill fraction of metal is influencing the reflectance effect of single ARC. It was found that the hfO₂SLARC on Si wafer presented the lowest reflectance less than 1% in 400-600 nm wavelength range compared with bare silicon wafer.

The Ag/Ni/Co doped HfO₂ SLARC are also effectively acted as a potential SLARC with less than 0.5% reflectance at 550 nm wavelength. The low reflectance improve the absorbed Photon flux from 1.5 $*E^{21}$ to 3.2 $*E^{21}m^{-2}s^{-1}$. The results explores optimal Ag/Ni/Co doped HfO₂SLARC s on Si wafer achieved the low reflectance good optical properties as well as the importance of metal doped SLARC enhances surface, Mechanical, self-cleaning properties. Both bare HfO₂ and metal-doped HfO₂ are potential candidates for making inexpensive, highperformance Si solar cells. In order to improve efficiency, Co doped HfO₂ was determined to be the most suitable option, while Ni was discovered to be the second most affective dopant in HfO₂ among the dopants studied. Optical research has revealed a significant increase in optical conductivity and absorption in the higher photonic energy range, particularly for Co/Ni doped HfO₂.

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