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Optimization of the Refractive Index of Antireflection Coatings on Monocrystalline Silicon Solar Cells for Photovoltaic Application

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ABSTRACT

In this work, the following materials have been chosen as anti-reflection layer, namely hafnium (HfO2), magnesium fluoride (MgF2), silicon oxynitrides (SiOxNy), silicon oxides (SiOx), silicon nitride (Si3N4) and hydrogenated silicon nitride (SiNx:H). The calculations were made on the basis of values of layer thicknesses and refractive indices that allow the phase and amplitude conditions to be respected and amplitude conditions. Numerical simulations have shown that low reflectivities at the surface of the surface of the plane cell coated with a simple layer, can be obtained. For example, for simple coatings materials based on Si3N4 and HfO2, we obtain a value of reflectivity around 3 and 2 % respectively. The structures with multilayer coatings such as MgF2/SiNx:H/Si, give a reflectivity of around 1 %. Thus, the refraction index of the coating is an important parameter that plays a major parameter that plays a major role in the optical properties of materials. The closer the refractive index is close to the index of the substrate or the layer above the substrate, the higher the reflectivity.

Keywords: Anti-reflective coating, single layer, multi-layer, reflection, refractive index

Introduction

Energy production is a central issue in our societies, with repercussions at all levels (economic, geopolitical, environmental, social...). Energy is indeed consumed, in its various forms, by all sectors of activity. Solar energy is one of the sustainable, abundant and clean solutions. It is obtained by converting the sun's rays into electricity through silicon, on which there is a very high reflection of the incident ray, thus a high loss. In order to reduce the reflectivity, the use of an anti-reflection layer (CAR) is anti-reflection layer (CAR) was imposed.

Influence of the Refractive Index of the Anti-reflective Coating

The evolution of the reflection coefficient of a silicon solar cell has been examined in this section. The substrate is coated with a single layer of anti-reflection material. The materials considered are MgF_2 , Si_3N_4 , SiN_x : H, SiO_xN_y , SiO_2 , HfO₂, whose index and thickness values used for the calculation are listed table below at the reference length of 700 nm[1,2,3,4].

$\lambda_0 = 700 \text{ nm}$		
Materials	Refractive	Thickness
	indexes	(nm)
MgF_2	1,38	127 ,17
SiO _x	1,50	116,67
SiO _x N _y	1,80	97,22
Si ₃ N ₄	2,03	86,11
HfO ₂	2,10	83,37
SiN _x : H	2,30	58,33
Si	3,78	46,20
(substrat)		

Table .1 Materials used as anti-reflection layers with their refractive indices and optimum thicknesses for a reference wavelength $\lambda_0 = 700$ nm.

Fig.8 shows a variation of the reflectivity from 400 nm to 1000 nm for the various coatings of the solar cell, the minimal value is observed for the reference wavelength ref ($\lambda 0$) = 700 nm. It is observed, the structures Si3N4/Si, SiOxNy/Si and HfO2/Si, present a null reflectivity at the reference wavelength, knowing that for the monocrystalline silicon the reflectivity turns around 33 % at this same reference wavelength.

This shows the importance of the coatings which makes the reflectivity pass to a value almost null thus generating a rather important transmission within the cells with an anti-reflection layer[5,6,7,8].

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Fig.1: Reflection of antireflective single-wave structures on silicon (reference wavelength 700 nm)

Beyond the reference wavelength, the reflectivity varies between 1 and 33% for all the different types of antireflective coatings.

The decrease in reflectivity for the three coatings mentioned above is due to the fact that these materials have refractive indices very close to the optimal index n = 1.96 ($nSiO_xN_y = 1.80$, $nSi_3N_4 = 2.03$, $nHfO_2 = 2.10$) and which correspond to the condition of obtaining destructive interference between the rays reflected by the coating. The transmission of the photon flow within the cell is thus improved.

However, the other coatings whose refractive indices present a deviation from the optimal index, the N conditions of destructive interference are not achieved. The optical path is much weaker, which leads to a decrease in reflectivity within the cells with anti-reflective coatings. The influence of the refractive indices shows the importance of the choice of the material as antireflection layer.

Study on Double Layer Anti-reflective Coatings

Research of the Best Configuration for Double Layers

The different anti-reflective materials used in this work will allow us to see their influence on different structures, namely coatings with decreasing refractive indices from the substrate (n = 3.78) to the ambient medium, the air (n=1).

The study in simulation is made by considering the materials of **Table. 1** coupled two by two in order to seek the best configuration of double anti-reflection layer[9,10,11].

Reflection Coefficient of an Anti-reflection Double Layer (SiO_x/HfO₂) on Silicon

The variation of the reflection coefficient of the double anti-reflection layer (DARC) with SiO_x and HfO_2 materials) is calculated in the wavelength range 400 nm - 1000 nm and plotted in Fig. 2.



Fig. 2: Reflectivity of DARC SiOx/HfO2/Si and HfO2/SiOx/Si structures.

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The study was made on two configurations namely the SiOx/HfO₂/Si and HfO2/SiOx/Si structures. The SiOx/HfO₂/Si structure, (whose material indices are in the order of 1.50, 2.10 and 3.78) shows a reflectivity of 10% at the reference wavelength. For the HfO₂/SiOx/Si structure (with material indices in the order of 2.10, 1.50 and 3.78), where the anti-reflection layers have been inverted, the reflection coefficient reaches 60%. This reflects the importance of the order in which the anti-reflective materials are deposited on the substrate; it is, therefore, necessary to deposit the layers in decreasing indices from the substrate to the top layer.

The fig. 3 also shows that single-layer coatings perform better at the reference wavelength. However, the two-layer coatings show zero reflectivities at 450 nm for the $HfO_2/SiO_x/Si$ structure and 500 nm for the $SiO_x/HfO_2/$ structure closer to the reference wavelength. This shift of the minimum reflectivity towards short wavelengths could be due to the fact that the juxtaposition of the two layers modifies the optical path of the waves in the materials. This leads to a change in phase that corresponds to destructive interference at another wavelength.

Reflection Coefficient of a SiOxNy / Si₃N₄:H Antireflection Double Layer on Silicon

The curves of fig. 3 represent the variation of the reflection coefficient of a DCAR ($SiOxNy/Si_3N_4$:H) according to the wavelength.



Fig.3: Reflectivity of DARC SiOxNy/Si₃N₄/Si and Si₃N₄/SiOxNy/ Si structures.

The value of the reflection coefficient for both structures is obtained at wavelengths between 450 and 500 nm, while it becomes maximum at the reference wavelength. The same behavior observed in the previous section is noted here also when reversing the order of deposition of the AR layers.

Reflection Coefficient of an Antireflection Double Layer (MgF₂/SiNx:H) on Silicon

The same observations and remarks of the two previous sections are noted in the case of the $MgF_2/SiNx$:H/Si and SiNx:H/MgF₂/Si structures (see Fig. 4 and 5).



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Fig. 4. Deflectivity of structures MgE /SiNy, U/Si et	Fig 5. Deflectivity of structures MgE /SiNy, U/Si et
Fig. 4. Kenecuvity of structures Mgr ₂ /Sinx. H/Si et	Fig.5. Reflectivity of structures Mgr ₂ /Sinx. fr /Si et
SiNx:H/MgF ₂ /Si.	SiNx:H/MgF ₂ /Si.
Index $n = 2$ pour le SiNx:H	Index $n = 3$ pour le SiNx:H

The observation of these two graphs, in relation to the increasing or decreasing order of the refractive indices and the change of refractive index of the SiNx:H material, (n = 2 then n = 3), largely shows the influence of the refractive indices and the order in which the materials are deposited. The reflectivity is minimal in the structure with decreasing refractive indices from the substrate to the top layer (MgF₂/SiNx:H/Si).

In the case of the SiNx:H/MgF₂/Si structure, and referring to Fig. 4 and 5, the reflectivity increases from 60 to 80% in the visible spectrum from 650 nm to 750 nm by taking the values of refractive index n = 2, then n = 3, respectively. This shows that the greater the difference between the indices of the anti-reflective layers, the higher the reflection for that where the top layer at a higher index. The opposite is observed for the MgF₂/SiNx:H/Si structure for which the change of the index of SiNx:H from n = 2 to n = 3, gives a variation of the reflectivity of 8% to 2% at the reference wavelength. This is compounded by almost no reflectivity in a longer wavelength range of 650 to 750 nm.

Variation of the Refractive index of One of the Antireflection Layers

Fig. 6shows the theoretical calculations developed for a material of variable refractive index and forming an intermediate layer between the substrate (Si) and the magnesium fluoride (MgF₂) of index n = 1.38[12,13,14,15].



Fig. 6: Variation of the refractive index of an antireflective layer as a function of wavelength.

For the simulations, the material index is taken between the values of the refractive index of MgF2 (n = 1.38) and n = 3. The decrease of the reflection coefficient as a function of wavelength is observed when the material index increases. At the same time, it is observed that the wavelength range for which the reflectivity is zero, becomes wider as the index increases.

Conclusion

This article was devoted to the simulation of anti-reflection layers involving, the best anti-reflection materials and the optimization of their performance. Anti-reflection layers play an important role in reducing optical losses in silicon solar cells which is a highly reflective material (60% loss of incident light flux). The variety of materials that can be used as anti-reflection layers provides several solutions. Among these different materials, magnesium fluoride (MgF₂), silicon nitride (Si₃N₄) and silicon oxide (SiO₂), have shown interesting properties by reducing to less than 35% the reflectivity of silicon. The closer the index of the layer is to the optimal index nair × nsilicon, the more the reflectivity becomes practically zero in the spectrum centered around the reference length that has been chosen in this work equal to 700 nm. Because of their respective properties, the combination of these materials in double layer, can be exploited to reduce both optical losses and losses related to recombination of minority carriers on the front side by passivation. Theoretical analysis has shown that a combination of two materials with appreciable index differences reduces the reflectivity of silicon over a wide spectral band as in the case of the double layer coating MgF₂/SiNx:H/Si whose indices are respectively 1.3767 and 2.3000. On the other hand, if the values of

the indices of the materials of the double layer are very close, the reflectivity becomes important in the part of the spectrum centered around the reference wavelength.

The option of making anti-reflection coatings to reduce photon losses at the surface of silicon, obeys certain conditions. It requires the development of calculation models, allowing to take into account the components of the different media (air / antireflection / silicon). The matrix approach is more general and allows to treat several layers, including interfaces. However, it is necessary to find a good compromise between the thickness of the AR layer to be deposited on the substrate and the adequate material to obtain the minimum of reflection in the active area of the silicon.

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