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Zinc Oxide Sub-Wavelength Structures as Antireflective Layer for Crystalline Silicon Solar Cells

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Abstract

The surface reflectance spectra of the zinc oxide (ZnO) sub-wavelength structures (SWSs) are investigated by using the rigorous coupled wave theory. And the effective reflectance of ZnO SWS is calculated for the standard solar spectrum over the wavelength range from 400 nm to 1000 nm. It is found that a lowest effective reflectance of 0.62% can be obtained for the optimized ZnO SWS, which is much less than that (5.94%) of an optimized ZnO single layer antireflection coatings (80 nm). A 10.0-μm-thick c-Si solar cell efficiency with the optimized ZnO SWS exhibits a 1.03% improvement than that of ZnO single layer antireflection coatings. It is demonstrated that lower reflectance of the ZnO SWS across solar spectrum has potential application in solar cell industry.

***Keywords**: ZnO, sub-wavelength structures, antireflection coatings, rigorous coupled wave theory, crystalline Si solar cells*

1. Introduction

The Fresnel reflection of incident light is always existent on an interface between two different transparent media. A beam of light from air impinges on the surface of high index of refraction crystalline Si, it will cause a great deal of photons to be reflected back from the interface. There is an effective method to reduce the number of lost photons by a substrate covered with single layer antireflection coating (SLARC) [1, 2]. However, it is not able to cover a wide range of the solar spectrum. In recent years, multilayer antireflection coatings have been studied which can fulfill wide wavelength range than SLARC [3-6]. Unfortunately, it is very difficult to associate with the different coating materials well and various physical-chemical properties will result in some problems, such as adhesion, thermal mismatch and the stability of the thin-film stack [7]. As is well known, the sub-wavelength structure (SWS) with feature size smaller than the incident wavelength is one of the best candidates to reduce the reflection of incident light in a broad range of the solar spectrum. Thus, some SWSs based on optical characteristic have been proposed for solar cells applications. For example, the effective reflectance of pyramid-shaped Si_3N_4 SWS has been analyzed by using a rigorous coupled-wave approach over the wavelength range from 400nm to 1000 nm [8]. And then, the effective reflectance of the Si_3N_4 SWS, which comprise a Si_3N_4 layer superimposed an etched Si_3N_4 grating with the cross-section of the strip in triangular shape, has also been studied using finite element analysis [9]. The results show that the lowest effective reflectance of the optimized Si_3N_4 SWS is 1.98%. In addition, a reflectivity below 1% is observed from 300 nm to 1000 nm for Si pyramid-shaped SWS grating which is approximated by a stack of 8 or 16 layers of Si slabs [10]. Here, a new kind of zinc oxide (ZnO) SWSs are proposed for crystalline Si solar cells applications, which mainly contain an etched ZnO

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layer on the bottom of an superimposed ZnO grating with the cross-section of the strip in multilevel surface profile.

In this study, we numerically examine the reflection characters of ZnO SWSs, which are optimized to get the lowest effective reflectance. And then, The ZnO SWS with the lowest effective reflectance are applied to a 10.0-μm-thick c-Si solar cell for estimating the electrical characteristics of a p-n junction solar cell. Finally, the solar cell efficiencies for ZnO SWS, bare sillion and ZnO SLARC are also compared and discussed.

2. Structure and Simulation

The proposed schematic diagram of the three-dimensional (3D) ZnO SWS is shown in Figure 1, which is composed of an etched ZnO and a ZnO grating with the cross-section of the strip in multilevel surface profile. The multilevel grating constituted by a stack of 9 layers of ZnO slabs with identical height is unlimited extension of the *x*-axis direction and reduplicate periodicity in the *y*-axis direction. The calculation parameters are defined as the period *Λ*, the height *h*, the top width *a*, the bottom width *b* of the etched ZnO grating and the thickness of the ZnO layer to be *t*. In order to examine conveniently the effect of different width intermediate layers in the ZnO SWS, here we assume the width difference between neighbouring layers is *d*. So, the numerical relations between *a* and *b* can be expressed as $b=a+8d$.

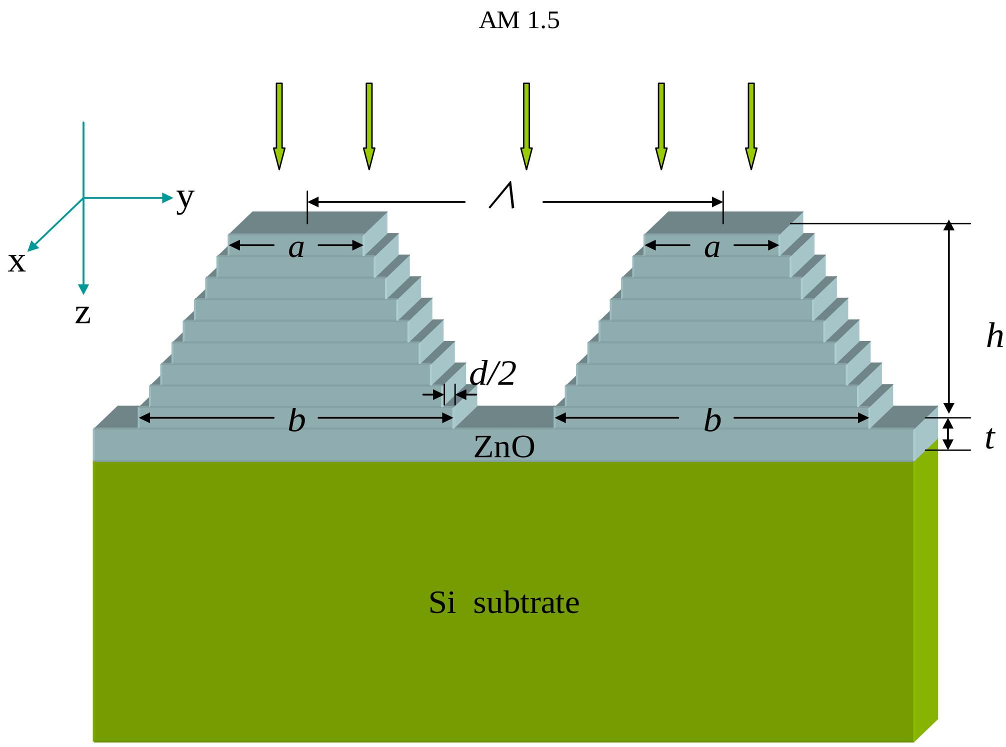

Figure 1.The Schematic Diagram of the Proposed ZnO SWS Structure, Where is the Period *Λ*, *H* is the Height, *A* is the Top Width, *B* is the Bottom Width, *D* is the Width Difference of Border Upon Layers of the Etched ZnO Grating and *S* is the Thickness of the Zno Layer

The refractive index of ZnO in our model is the same with that used in [11]. In addition, an empirically fitted formula for the wavelength dependent of n_{Si} is employed in our simulation program [12].

$$n_{\mathrm{Si}} = \sqrt{\sigma + \frac{A}{\lambda^2} + \frac{B\lambda_1^2}{\left(\lambda^2 - \lambda_1^2\right)}} \quad (1)$$

Where σ=11.6858, A=9.39816×10^{-12} m^2, B=8.10461×10^{-3}, and λ=1.1071×10^{-6} m. The effective reflectance (R_{eff}) for ZnO SWS is determined by the following equation [13].

$$R_{\mathrm{eff}} = \frac{\int_{\lambda_1}^{\lambda_2} R(\lambda) N_{\mathrm{ph}}(\lambda) \mathrm{d}\lambda}{\int_{\lambda_1}^{\lambda_2} N_{\mathrm{ph}}(\lambda) \mathrm{d}\lambda} \quad (2)$$

Where, λ is the light wavelength; λ_1 and λ_2 are the lower and upper wavelength of the spectrum range. Here, λ_1=400 nm and λ_2=1000 nm for the AM1.5 solar illumination; $R(\lambda)$ is the spectral reflectivity of the light; and $N_{\mathrm{ph}}(\lambda)$ is the photon number of the light with the wavelength λ in the AM1.5 solar illumination [14].

When the sunlight, which can be approximated by a plane wave, is incident on the front surface of ZnO SWS, $R(\lambda)$ can be calculated by the rigorous coupled wave theory [15]. In addition, the incident light will propagate through the medium in a straight direction when the period of SWS is much less than the wavelength of the light [16]. Therefore, we merely study the reflectivity without considering the diffraction orders in this work. The initial parameter of ZnO SWS values in our simulation are summarized in Table 1.

Table 1. Some Initial Values for the ZnO SWS Parameters in the Simulation

Parameters	Value
The grating period Λ (nm)	200
The grating depth h (nm)	150
The thickness of the ZnO layer t (nm)	70
The bottom width of the grating b (nm)	90
The thickness of border upon layer d (nm)	5

3. Result and Discussion

3.1. Surface Reflection

Firstly, the surface reflectance of the ZnO SWS is calculated for several different heights h as a function of incident wavelength over the wavelength range from 400 nm to 1000 nm in Figure 2. One can see that the reflectance is decreased with increasing the height of SWS in the whole visible region (*e.g.*, a nearly flat curve at h=135 nm). On the other hand, the reflectance is undulate in creased with the increase of the wavelength when the height of ZnO SWS is over 135 nm. And, the reflectance is increased with increasing the height for the wavelength ranging of 750 nm to 1000 nm. Hence observations suggest that it is significant to discuss the proper height of ZnO SWS for the lowest reflectance.

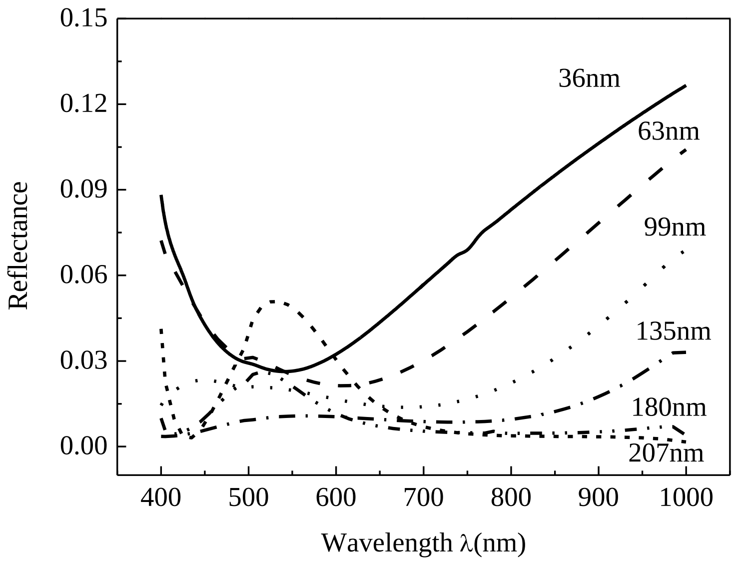

Figure 2. Calculated Reflectance of ZnO SWS for the Several Heights as a Function of Incident Wavelength

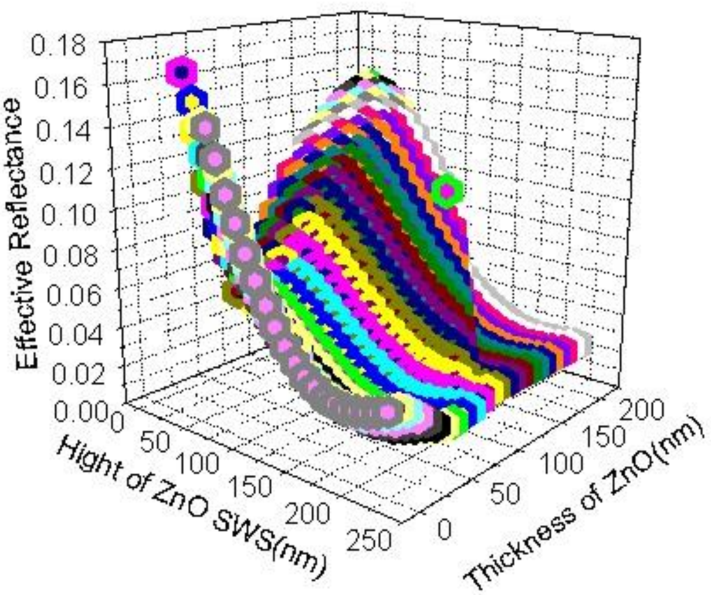

Figure 3. The Effective Reflectance Versus the Thickness of ZnO(*S*) and the Height of ZnO SWS (*H*)

Thus, considering preferential the parameters for ZnO SWS in the *y*-axis direction, the effective reflectance of ZnO SWS is calculated for variety of *h* and *s*, where other parameters from Table 1. The results is shown in Figure 3; from which one can see that the lowest of R_{eff}=0. 75% occurs at *h*=171 nm and *t*=65 nm.

Figure 4 generalizes the lowest effective reflectance for the several *d* as a function of *a*, where *h*=171 nm, *t*=65 nm over the same wavelength range. It is shown that the effective reflectance firstly decreases and then increases as the increasing *a*, whatever the value of *d*. On the other hand, the larger *d* (from 3 nm to 9 nm), the smaller *a* for the lowest effective reflectance. There is a minimum R_{eff} (0.625%) for *a*=55 nm and *d*=5 nm. And, it is obvious that *b*=95 nm from the equation for previous description in this study.

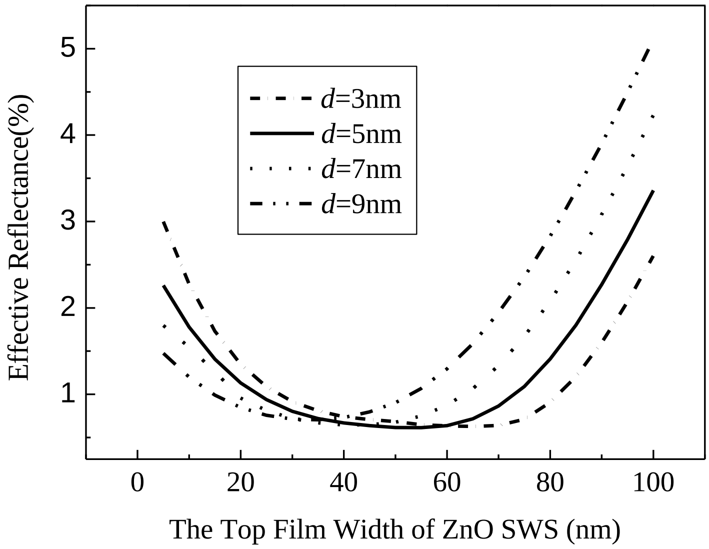

Figure 4. The Effective Reflectance for the Wavelength for the Varying to 1000 Nm: Plot is As *A* Function of *A* and *D* For ZnO SWS

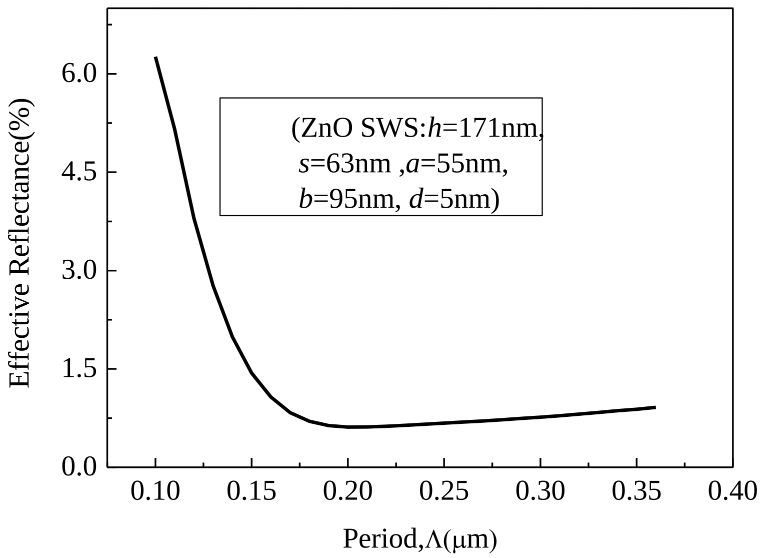

Figure 5. The Relation between the Effective Reflective R_{eff} and Λ

We examine the effective reflectance of the ZnO SWS by varying Λ which is equal to a unit cell width. In Figure 1, the minimum value of Λ is equal to the bottom width *b* (95 nm), so we change the unit cell width Λ from 100 nm to 300 nm and fix the *h*, *t* and *d* at 171 nm, 65 nm and 5 nm, respectively. The relation between the effective reflective and Λ is shown in Figure 5. It can be seen that the effective reflective drops intensely as Λ from 100 nm to 150 nm and then varies a little increscence. The minimum of R_{eff} is attained for Λ=200 nm.

In the end, the lowest effective reflectance of R_{eff}=0.613% can be obtained with the optimized ZnO SWS, where *h*=171 nm, *t*=65 nm, *a*=55 nm, *d*=5 nm, and Λ=200 nm. The effective reflectance of the optimized ZnO SWS, bare sillion and 80 nm ZnO SLARC in the wavelength ranging of 400 nm to 1000 nm are tabulated in Table 2. From Table 2, it is clear that the ZnO SWS has the lowest effective reflectance of 0.613% as compared to bare sillion, 80 nm ZnO SLAR coating. The spectral reflectivity of the optimized ZnO SWS, bare sillion and 80 nm ZnO SLARC over the wavelength ranging of 400 nm to 1000 nm are shown in Figure 6. It is found that the spectral reflectivity of ZnO SWS is lower than that of ZnO SLARC except a pimping section for the wavelength range of 600 nm to 700 nm.

Table 2. Effective Reflectance for the Optimized Structures of ZnO SWS, Bare Sillion and 80 nm ZnO SLARC for the Wavelength Range from 400 nm to 1000 nm

Structure	Effective reflectance (%)
Bare Sillion	21.21
ZnO SLARC	5.94
ZnO SWS	0.613

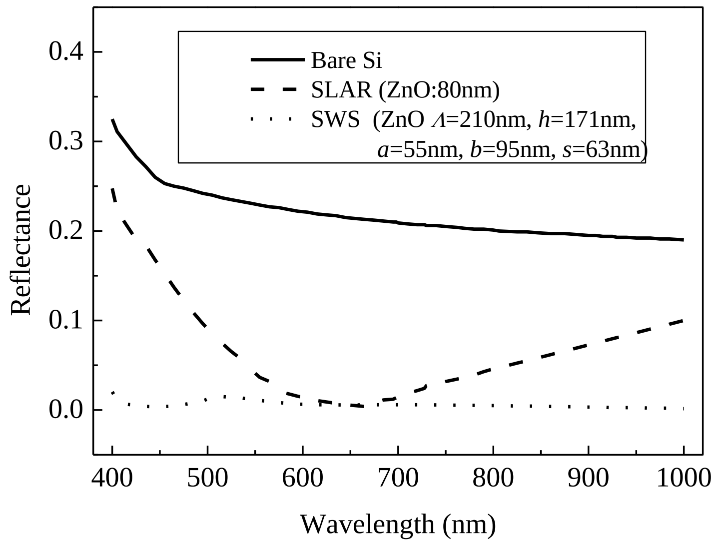

Figure 6. The Spectral Reflectivity of the Optimized ZnO SWS, ZnO SLARC and Bare Si

3.2 The SWS for Solar Cell Applications

As a example, a 10.0-μm-thick c-Si solar cell model is applied to examine antireflective properties of zinc oxide sub-wavelength structure. The total efficiency of the solar cell can be calculated by:

$$\eta = J_{sc} V_{oc} FF / P_{in} \tag{3}$$

where J_{SC}(A/cm^2) is the short-circuit current density, V_{OC}(V) is the open-circuit voltage, FF is the fill factor, and P_{in} is defined as the incident power (P_{in}=0.1w/cm^2 under illumination AM 1.5).

$$J_{SC} = \int_{\lambda_1}^{\lambda_2} e\eta_c A(\lambda) N_{ph}(\lambda) d\lambda \tag{4}$$

where e is the election charge, $A(\lambda)$ is the absorptance for each wavelength which can be calculated by RCWA [15]. The collection efficiency (η_c) of Si material is assumed to be a constant 85%, which means that 85% of the incident light would be absorbed to generate electron-hole pairs [17].

$$V_{oc} = (kT/e)\ln(J_{sc}/J_{so} + 1) \tag{5}$$

Where k is the Boltzmann's constant, T=300 k and J_{so} is reserse bias saturation current (1.5×10^{-11} A/cm^2). As for the fill factor, FF=80% is that can be achieved with adequate choice of a load. In addition, the external quantum efficiency (EQE) is calculated by [18]

$$EQE(\lambda) = A(\lambda)\eta_c \tag{6}$$

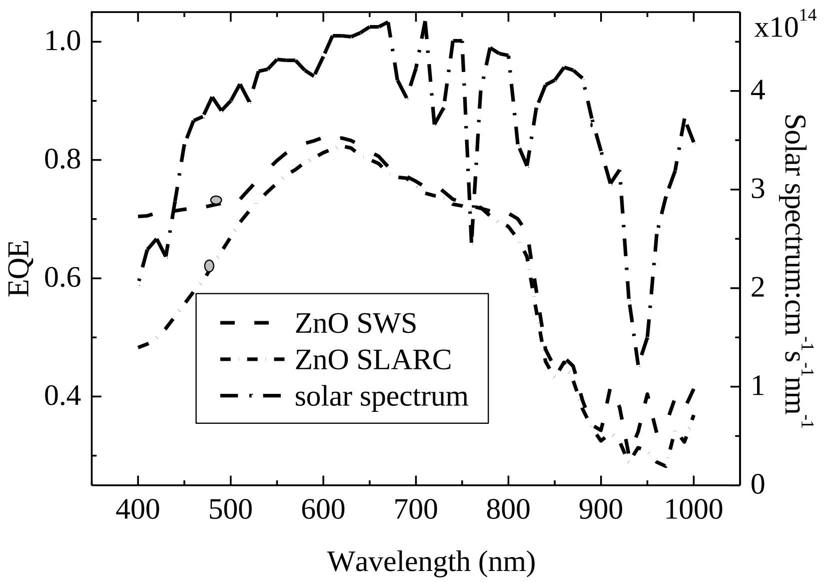

Figure 7. External Quantum Efficiency as a Function of Wavelength for 10-μm-Thick Si Solar Cell

Table 3. The Electrical Characteristics of 10-μm -thick Si solar Cell with Different Surface Structures

Structure	J_{sc} (mA/cm^{-2})	V_{oc}(mV)	Efficiency (%)
Bare Sillion	22.34	0.5471	9.77
ZnO SLARC	33.12	0.5568	14.75
ZnO SWS	35.38	0.5583	15.78

The electrical characteristics of 10-μm-thick Si solar cell with different surface structures are shown in table 3. The solar cell efficiency with the optimized ZnO SWS exhibits a 1.03% improvement than that of ZnO single layer antireflection coatings. External quantum efficiency as a function of wavelength for 10-μm-thick Si solar cell is shown in Figure 7. The thick cell (t=10 μm) of the ZnO SWS structure brings considerable absorption enhancement almost in the wide wavelength range of 400 nm to 1000 nm.

4. Conclusion

In this paper, we have calculated the surface reflectance spectra of the indium tin oxide (ZnO) sub-wavelength structure (SWS). The effective reflectivity of ZnO SWS over the wavelength range from 400 nm to 1000 nm for standard solar spectrum is computed. Results of our study indicate that a lowest effective reflectivity of 0.613% can be obtained for the computed ZnO SWS with h=171 nm, t=65 nm, a=55 nm, d=5 nm and Λ=200 nm, which is much less than those obtained an optimized 80 nm ZnO SLARC (5.94%). In order to estimate the reflective effect of optimized ZnO SWS, a 10.0-μm -thick c-Si solar cell efficiency based on the optimized ZnO SWS is also calculated, resulting an improvement of 1.03% efficiency than those of single layer antireflection coatings.

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