Linear Graded Refractive Index Antireflection Coatings
For Silicon Substrate

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Abstract
In this work, a theoretical study of linear profile for graded antireflection coating has been used with silicon as substrate. A computer program has been designated using the basic equations of thin film, and the reflectance has been obtained over a wide range of wavelengths (400-1000 nm) as well as incident angles (0-60 degree) for many film thicknesses. The film consist of hydrogenated nitrides, it was shown that the reflectance decreases as the thin film thickness increases. The reflectance reaches to less than 1% for thin film thickness 0.6 µm.

Keywords: Graded refraction index, Antireflection for solar cell, Graded thin layer.

Introduction
Measurements of reflectivity carried out in the ultraviolet, visible and near infrared range show that the graded refractive index thin films could be used as antireflection coatings for silicon solar cells. The reducing of the reflection of surfaces by using antireflection material has considered to be an important aim to improve many optical components. The antireflection coatings can be classified into two types depending on their structure, the homogeneous layer or step index coating and inhomogeneous layer or graded index coating.

For step index coatings, the material and thickness of the layer have to be chosen carefully for each wavelength, angle, and substrate. The width of these coatings is lower than one micron, for example, 400–700 nm or 800–1100nm, and the angle of incidence is limited to 30 degree [1].

The refractive index for inhomogeneous coatings (with gradient-index) varies gradually and monotonically along its thickness from the ambient (usually air) index to the

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substrate index [2]. Comparing with multilayer uniform films, gradient-index antireflection coatings can be less sensitive to the angle of incidence [3], and is thus desirable for use in many applications.

The refractive index of the AR coating is constrained by the availability of materials with refractive indices matching the substrate and the ambient. That is, for an infinitely thick, continuously graded AR coating, Fresnel reflectivity approaches zero.

A linear profile is a reasonable starting point, but other profiles, Quintic, Gaussian, Exponential, Exponential-Sine and Klopfenstein [4-7], the quintic profile, have been found to give superior performance.

Approximating our step-graded refractive index profile with a continuously graded profile has been confirmed to worsen the reflection properties of the AR coating, i.e., the interference effects that continuously graded coatings expressly avoid, are weakened. This result is relevant to virtually all thin film coatings that have practical uses in photonics applications. Specifically, it applies to common components such as solar cells, sensors, detectors, lenses, and solid-state lighting devices. It has been considered that the light incident from a low-refractive-index ambient upon a high refractive index substrate.

The transmittance [8] of Si emission at the Air-Silicon is low due to the large refractive index discontinuity that exists at the Air-Silicon range. By placing a single layer antireflection coating of intermediate refractive index on the Silicon surface, this large index discontinuity is broken into two smaller steps, resulting in a lower broadband reflectivity. Further reduction in broadband reflectivity can be achieved by adding additional intermediate index layers, thus breaking the air-Silicon index discontinuity into smaller and smaller steps. Therefore, a gradient index AR is the limit of this progression, where a single index discontinuity is replaced by a continuous transition from a high to a low index material (air), if this continuous index transition occurs over several wavelengths of optical path length, broadband reflectivity approaching zero can be achieved [9].

Recently, oblique-angle deposition has been used to demonstrate nano porous films with a refractive index approaching that of air. These nano porous films are stable, showing no signs of deterioration over time or in response to aqueous environments. Besides allowing very low refractive index values, oblique-angle deposition and other techniques can be used to precisely tune the refractive index within a broad range by varying a material’s porosity [10].

Researchers at Rensselaer have discovered several improved designs and methods for increasing the performance of antireflection coatings, including:

Broadband elimination of Fresnel reflection through the use of TiO$_2$ and SiO$_2$ nano rod layers (by oblique angle deposition), where the refractive index is controlled down to a minimum value of $n = 1.05$ [11, 12]. The new designs and selection principle of gradient-index antireflection coating profiles leading to a decrease in overall reflection at various angles of incidence without extending the film’s thickness. To reduce the reflection of the solar cell, the surface of the solar cell is texturized before depositing the AR coating, mainly in silicon technology.
These modern coatings with hydrogenated silicon nitrides (SiN:H) are very appreciated because of their passivation properties [13].

In this research, a thin film has a graded refractive index ranging between the air refractive index (1.0) and substrate (silicon) refractive index (3.91) at wavelength (700 nm)[14] used theoretically to minimize the reflection spectrum via the wavelength range (400-1000 nm). The antireflection coating consists of a dense TiO$_2$ and two nanoporous SiO$_2$ layers fabricated using oblique angle deposition [15].

**Mathematical form of the optical system**

The geometry of a gradient-index antireflection is shown in Fig. 1. The inhomogeneous film is placed on a silicon substrate with an index (3.91), and the ambient is assumed to have an index (1.0). The ambient-film interface is at $z=0$ while the film-substrate interface is at $z=d$, where $z$ is the physical distance normal to the film surface. Inside the film the refractive index $n(z)$ varies continuously from (1.0) to (3.48) linearly. All media are assumed to be non dispersive and non-absorbing.

The mathematical reflectance ($R$) and transmittance ($T$), which measure the energy reflected from/or transmitted through the film, respectively, are given by [16]:

$$R = \frac{|(Er)_{j+1}|^2}{|Et_{j+1}|^2} \text{ ......................... (1)}$$

$$T = \frac{n_m}{n_o} \frac{1}{|(Et)_{j+1}|^2} \text{ ......................... (2)}$$

$(Er)_0$ and $(Et)_0$ are the reflected and transmitted electric field amplitudes at the incident medium, respectively. $(n_0)$ and $(n_m)$ are the refractive indices of the incident medium and substrate, respectively. The basic recursion relation for the reflected and transmitted electric field amplitudes for all layers is:

$$\frac{(Et)_{j+1}}{(Er)_{j+1}} = \frac{1}{2} \left( \frac{1 + \frac{n_j}{n_{j+1}} e^{i\phi_j}}{1 - \frac{n_j}{n_{j+1}} e^{i\phi_j}} \right) (Et)_{j} \text{ ........................................ (3)}$$

$$\phi_j = \frac{2\pi}{\lambda} n_j d_j \text{ ......................... (4)}$$

($n_j$ and $d_j$) are the refractive index and the thickness of layer $(j)$ of the coating system. $\phi_j$ is the phase difference of the layer $j$. The procedure to compute the reflectance or the transmittance for the multilayer system is to apply equation (3) recursively, starting at the bottom-most layer, i.e., $j=m$ (substrate), backward to layer $j=0$ (incident medium).

The spectral reflectivity $R$ will be calculated using the characteristic matrix method (equation 3) considering the graded film as a superposition of fixed refraction index sub-layers with the same thickness. The film layer has been divided to 100 sub layer; each one has same thickness in a way that the total thickness must equal to film thickness.

**Results**

A computer program has been designated using the basic equations of multilayer thin films (equations 1-4), the program can reach to the best design that achieve the designer requirements such as minimum reflectance within given band of wavelengths.

The reflectance was calculated between 0.4 and 1.0 µm as shown in Fig. (2). The dot line represents the best design of step index thin film deposited on silicon substrate in order to have minimum reflectance at the
whole range of wavelength, the results of the using program gives film with refractive index (1.8655) and thickness (0.08059 µm).

The solid lines in Figure (2) represent the reflectance for many layer thicknesses (0.08 to 0.6 µm). It shows the significant reduction due to the presence of graded index antireflection coating, the mean reflectance decreases from 17.1% to 1.0%.

Figure (3) shows the mean reflectance over the whole range of wavelength as a function for film thickness, it is obvious that the reflectance decreases as the thin film thickness increase.

All the above results have been achieved for normal light incident, but for other incident angle the reflectance spectrum will vary to high values. To illustrate the effect of the incident angle for arbitrary thin film thickness (such as 0.6 µm), Figure (4) shows that the mean reflectance difference is very small for incident angle less than 20°, and is equal to about 16 % for incident angle 30°.

Conclusions

It has been demonstrated that the newly linearly graded thin film systems can be optimized to provide better antireflection coatings. The thin film coating has been simulated to obtain the reflectance as a function of wavelength and incident angle. The reflectance decreases as the thin film thickness increases, thus the controlling of the reflectance can be achieved via controlling thin film thickness. The reflectance can reach to less than 1 % for thickness 0.6 µm. Increasing the thin layer thickness to more than 0.6 µm will decrease the reflectance to less than 1 %. But the experimental difficulty to manufacture graded index thin film is still the main restriction. However the graded dielectric materials promise excellent antireflection properties and have been the subject of scientific analysis and investigation.

References


Figure (1): The refractive index profile of the optical system (ambient, thin film, substrate)

Figure (2): The reflectance spectrum for different graded thin film thicknesses. The dot line represents the reflectance spectrum for the case of step index.
Figure (3): The mean reflectance at the whole wavelength range for different thin film thicknesses.

Figure (4): The reflectance for thin film thickness (0.6 µm) for different incident angle.