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Effects of Thin Films' Number on Nano Scale Radiative Properties

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Abstract: Many of optical components and semiconductors coated with thin films, so study of thin film coating is very important for industries. This work uses transfer-matrix method for calculating the radiative properties. Lightly doped silicon is used and the incoherent formulation is applied. The empirical expressions for the optical constants of lightly doped silicon are employed. Silicon dioxide and silicon nitride are used as thin film coatings. It is possible to choose the suitable coating for maximum emittance, minimum transmittance and or minimum reflectance. It depends on industrial usages. This paper considered effects of thin films' number with various compositions of coating materials (9 cases). High emittance is needed for suitable thermal balance of the thin-film solar cells for space applications. Optical coatings that provide high emittance must be formed on the solar cells to overcome that problem by increasing number of thin film layers. Radiative properties are complex function of wavelength. Increasing number of thin film layers lead to more complexity and dependency on wavelength regard to wavelength interferences. Results showed that increasing number of thin film coating is more effective on radiative properties than increasing thickness. For example in the constant total thickness, it is possible to reach greater emittance by increasing layers' numbers. From results, the average emittance for bare silicon from 0.0499 reaches to 0.1725 with coatings in case number 9.

Key words: Thin Films % Number % Different Coatings % Reflectance % Emittance % Transmittance

INTRODUCTION

Optical techniques and radiative processes play important roles in current industry and daily life. Examples are advanced lighting and display, materials and surface characterization, real time processing monitoring and control, laser manufacturing, rapid thermal processing (RTP), communication, data storage and reading, radiation detection, biomedical imaging and treatment, ground and space solar energy utilization, direct energy conversion, etc. Optical and thermal radiative properties are fundamental physical properties that describe the interaction between electromagnetic waves and matter from deep ultraviolet to far-infrared spectral regions [1].

Surface modification by coatings can significantly affect the radiative properties of a material [2]. In fact, surface modification by coatings can significantly affect the radiative properties of a material [1-4]. It is observed that the concentrations highly affect the radiative properties of doped silicon multilayer at temperatures below 600 K. At temperatures below 600 K the concentration and the type of impurities have important effects on the radiative properties of the film. Moreover, the effects of ions are considerable for the concentrations higher than 10^{16} cm^{-3} [3]. Silicon dioxide and silicon nitride coating act as anti reflector and these coatings reduce reflectance toward bare silicon. If thickness of non metal coating increases, reflectance of multilayer decreases and transmittance increases. Gold thin film coating increases reflectance. The reflectance of multilayer coated with gold increases by increasing the thickness of coating [4].

Thin film coatings play an important role in the semiconductor industries and micro electromechanical and nano electromechanical equipments. Increasing of non metal thin film coating's thickness greater than 100 nm causes increasing of transmittance and decreasing of reflectance rapidly. Reflectance increases and transmittance decreases rapidly till thickness of gold thin layer reaches to 60 nm [5]. The difference between S-polarization and P-polarization increases with increasing

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of incidence angle. The reflectance of S-polarization is greater than the reflectance of P-polarization. When the incident radiation is unpolarized, the radiative properties are averaged over p and s polarizations. Thermal radiaitive properties of nanoscale multilayer structures strongly depend on impurity types and incidence polarization. Therefore industrial requirements are supported by selecting donors or acceptors and s or p incidence polarization [6]. When the film thickness increases, the free spectral range decreases, resulting in more oscillations with thicker silicon dioxide film. But interferences in the substrate are generally not observable in incoherent formulation [7].

This work uses incoherent formulation for calculating the radiative properties of semiconductor materials related to the recent technological advancements that are playing a vital role in the integrated-circuit manufacturing, optoelectronics and radiative energy conversion devices. Lightly doped silicon is used and the empirical expressions for the optical constants of lightly doped silicon are employed. Silicon dioxide and silicon nitride are used as thin film coatings. This paper considered effects of thin films' number with various compositions of coating materials (9 cases) that not been considered in perevious papers.

Modeling

Coherent Formulation: When the thickness of each layer is comparable or less than the wavelength of electromagnetic waves, the wave interference effects inside each layer play an important role in accurate prediction of the radiative properties of the multilayer structure of thin films. The transfer-matrix method provides a convenient way to calculate the radiative properties of the multilayer structure of thin films. Assuming that the electromagnetic field in the j_{th} medium is a summation of forward and backward waves in the z-direction, the electric field in each layer can be expressed by [1]:

$$E_j = \begin{cases} \left[A_1 e^{iq_{1z} z} + B_1 e^{-iq_{1z} z} \right] e^{(iq_x x - iwt)}, \; j = 1 \\ \left[A_j e^{iq_{jz}(z - z_{j-1})} + B_j e^{-iq_{jz}(z - z_{j-1})} \right] e^{(iq_x x - iwt)}, \; j = 2,3,...N \end{cases} \quad (1)$$

Here, A_j and B_j are the amplitudes of forward and backward waves in the j_{th} layer. Detailed descriptions of how to solve Eq. (1) for A_j and B_j is given in [1].

Incoherent Formulation: When the thickness of silicon substrate is much greater than the coherent length and the considered wavelength falls in the semitransparent region of silicon, interferences in the substrate are generally not observable from the measurements. In this case, the incoherent formulation or geometric optics should be used to predict the radiative properties of the silicon substrate. Two ways to get around this problem are to use the fringe-averaged radiative properties and to treat thin-film coatings as coherent but the substrate as incoherent [1]. Note that the transmittance J_i is the same when absorption inside silicon is negligibly small [8].

Detailed of incoherent formulation was discussed in [7]. The absorption of silicon can be taken into consideration by introducing the internal transmittance

$$t_i = \exp(-\frac{4p k_s d_s}{l \cos q_s}) \quad (2)$$

Here, k_s is the extinction coefficient of silicon, d_s is the thickness and 2_s is the angle of refraction. The angle of refraction is complex due to absorption. For a slightly absorbing medium with k_s —, however, 2_s can be determined using Snell's law by neglecting absorption [9]. Consequently, the radiative properties of the silicon wafer with thin-film coatings in the semitransparent region can be expressed as [10]:

$$r = r_{ta} + \frac{t_i^2 t_i^2 r_{bs}}{1 - t_i^2 r_{ts} r_{bs}} \quad (3)$$

$$t = \frac{t_i t_t t_b}{1 - t_i^2 r_{ts} r_{bs}} \quad (4)$$

$$e = 1 - r - t \quad (5)$$

Optical Constants

The Refractive Index of Silicon: The Jellison and Modine (J-M) expression of the refractive index for a wavelength between 0.4 µm and 0.84 µm is given in [11]. Li developed a functional relation, for the refractive index of silicon that covers the wavelength region between 1.2 µm and 14 µm [12]. The J-M expression is used in this study to calculate the refractive index of silicon for the wavelength region from 0.5 µm to 0.84 µm but Li's expression is employed for wavelengths above 1.2 µm. For a wavelength range of 0.84 µm to 1.2 µm, we use a weighted average based on the extrapolation of the two expressions.

The Extinction Coefficient of Silicon: The J-M expression of the extinction coefficient, covering the wavelength range from 0.4 µm to 0.84 µm, is given in [11]. The absorption coefficient can be deduced from the extinction coefficient. For longer wavelength regions, Timans suggested that the absorption coefficient can be expressed as a summation of the band gap absorption and free-carrier absorption as in the following [10]:

$$a(l,T) = a_{BG}(l,T) + a_{FC}(l,T) \quad (6)$$

The expression for the band gap absorption can be found in the work by MarcFalane *et al.* [13-14]. For free-carrier absorption, Sturm and Reaves suggested an expression [15]. Vandenabeele and Maex proposed a semi-empirical relation for calculating the extinction coefficient as functions of wavelength and temperature due to free-carrier absorption. The Vandenabeele and Maex (V-M) expression is given by [16]:

$$a_{FC}(l,T) = 4.15\times10^{-5}\, l^{1.51}(T+273.15)^{2.95}\exp\left(\frac{-7000}{T+273.15}\right) \quad (7)$$

Rogne *et al*. demonstrated that the absorption coefficient calculated from the V-M expression agrees well with experimental data for the wavelength region between 1.0 µm and 9.0 µm at elevated temperatures [17]. The optical constants of silicon dioxide are mainly based on the data collected in Palik [18].

RESULTS

Table 1 shows the used cases in order to comparing the radiative properties of nano scale multilayer. This paper considered the radiative properties of silicon coated with silicon dioxide and silicon nitride at room

Table 1: The Cases for comparing radiative properties

Case Number	Case Definition
1	Case 1:Bare Silicon with 700μm thickness
2	Case 2: Three Layers include Silicon substrate with 700μm thickness and coated with silicon dioxide with 300nm thickness from both sides
3	Case 3: Three Layers include Silicon substrate with 700μm thickness and coated with silicon nitride with 300nm thickness from both sides
4	Case 4: Five Layers include Silicon substrate with 700μm thickness and coated with silicon nitride on silicon dioxide with 300nm thickness from both sides
5	Case 5: Five Layers include Silicon substrate with 700μm thickness and coated with silicon dioxide on silicon nitride with 300nm thickness from both sides
6	Case 6: Seven Layers include Silicon substrate with 700μm thickness and coated with silicon dioxide on silicon nitride on silicon dioxide with 300nm thickness from both sides
7	Case 7: Seven Layers include Silicon substrate with 700μm thickness and coated with silicon nitride on silicon dioxide on silicon nitride with 300nm thickness from both sides
8	Case 8: Nine Layers include Silicon substrate with 700μm thickness and coated with silicon nitride on silicon dioxide on silicon nitride on silicon dioxide with 300nm thickness from both sides
9	Case 9: Nine Layers include Silicon substrate with 700μm thickness and coated with silicon dioxide on silicon nitride on silicon dioxide on silicon nitride with 300nm thickness from both sides

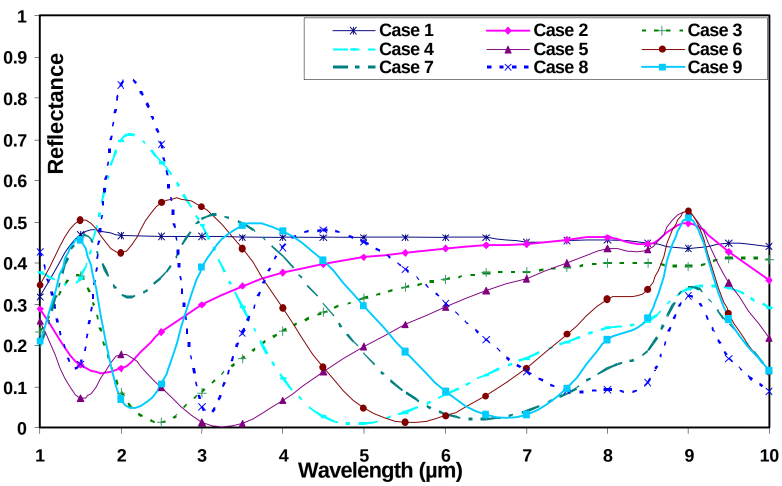

Fig. 1: A comparison of the spectral reflectance of different cases

Table 2: Comparison of average radiative properties for all cases

Radiative Properties/ Cases	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9
Average Reflectance	0.4494	0.3702	0.2968	0.2689	0.2436	0.2819	0.2399	0.2976	0.2489
Average Transmittance	0.5007	0.5202	0.6489	0.6206	0.6342	0.5626	0.6262	0.5367	0.5786
Average Emittance	0.0499	0.1096	0.0543	0.1104	0.1222	0.1556	0.1339	0.1657	0.1725

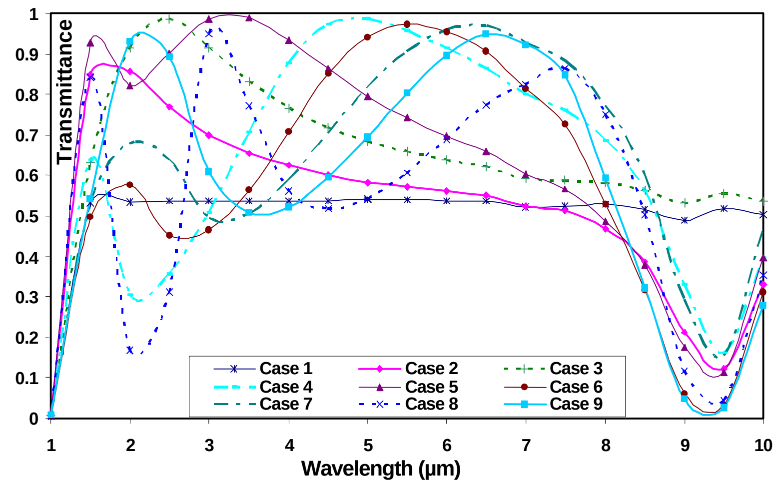

Fig. 2: A comparison of the spectral transmittance of different cases

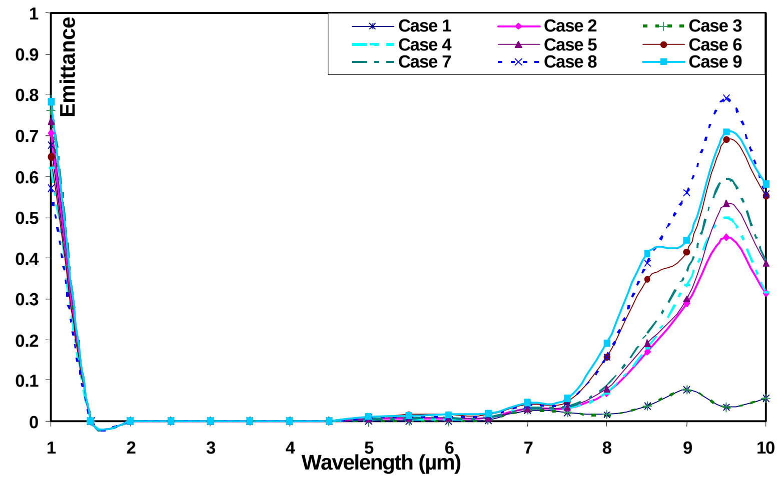

Fig. 3: A comparison of the spectral emittance of different cases

temperature for 9 layers with different coating procedures. The results for spectral reflectance are shown in Figure 1, spectral transmittance in Figure 2 and spectral emittance in Figure 3 for wavelengths between $1\mu m$ to $10\mu m$.

The fluctuations in the results are observed because of the wave's interferences, these fluctuations are in the shape of sinus curves and with increasing wavelength, the distance between peaks grows (Figures 1 to 3).

The average radiative properties consist of reflectance; emittance and transmittance are shown in Table 2.

CONCLUSION

From the Results:

- It is possible to choose the appropriate coating for maximum emittance, minimum reflectance and minimum transmittance.
- High emittance is needed for suitable thermal balance of the thin-film solar cells for space applications. It is possible to reach to this issue by increasing number of thin film layers.
- Increasing number of thin film coating leads to increasing the emittance that is due to waves' interferences in the layers.

- Radiative properties are complex function of wavelength. Increasing number of thin film layers lead to more complexity and dependency on wavelength based on wavelength interferences phenomena.
- Effect of increasing layers in order to controlling radiative properties is more than the effect of changing the thickness of layer. For example, it is possible to reach greater emittance by increasing number of coating layers in constant total thickness.
- The emittance of 9 coating layers is more than 7 coating layers, more than 5 coating layers, more than 3 coating layers and more than one coating layer.
- The average emittance for bare silicon is 0.0499. It reaches to 0.1725 by using thin film coating in case number 9.
- The reflectance in the wavelength $\lambda = 9.5\mu m$ decreases from 0.44899 to 0.1667 with selecting suitable coating. (By choosing coating of case number 8).
- The transmittance in the wavelength $\lambda = 9.5\mu m$ decreases from 0.5176 to 0.02585 with selecting suitable coating. (By choosing coating of case number 9).
- The emittance in the wavelength $\lambda = 9.5\mu m$ increases from 0.033 to 0.7898 with selecting suitable coating. (By choosing coating of case number 8).

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