World Applied Sciences Journal 9 (4): 372-379, 2010
ISSN 1818-4952

Comparison Radiative Properties of Thin Semiconductor Films by Coherent and Incoherent Formulation

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Abstract: Accurate radiometric temperature measurements of silicon wafers and heat transfer analysis of rapid thermal processing furnaces require a thorough understanding of the radiative properties of the silicon wafer, whose surface may be coated with dielectric or absorbing films. This Paper, predict the directional, spectral and temperature dependence of the radiative properties for the multilayer structures consisting of silicon and related materials such as silicon dioxide and silicon nitride. Results showed that for visible wavelengths, the reflectance decreases 60% as the coating thickness increases from 200 nm to 800 nm and the emittance increases 20% as the coating thickness increases from 200 nm to 800 nm. In these wavelengths, transmittance is negligible. In near infrared wavelengths, silicon nitride coating has higher average reflectance than silicon oxide coating and silicon dioxide coating has higher average emittance than silicon nitride coating. In visible wavelengths the reflectance increases as the temperature increases, because of decreasing emittance. Results showed that as 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.

Key words: Emittance % Reflectance % Transmittance % Incoherent Formulation % Coherent Formulation % Semiconductor % Multilayer

INTRODUCTION

Silicon is a semiconductor that plays a vital role in integrated circuits and microtechnology [1]. Semitransparent crystalline silicon solar cells can improve the efficiency of solar power generation [2]. Accurate radiometric temperature measurements of silicon wafers and heat transfer analysis of rapid thermal processing furnaces require a thorough understanding of the radiative properties of the silicon wafer, whose temperature and surface coated with dielectric or absorbing films. Accurate radiometric temperature measurements of silicon wafers and heat transfer analysis of rapid thermal processing furnaces require a thorough understanding of the radiative properties of the silicon wafer, whose surface may be coated with dielectric or absorbing films [1]. In fact, surface modification by coatings can significantly affect the radiative properties of a material [3].

Radiative properties of a material are the core of thermal science and optics, which play critical roles in modern technologies, including MEMS/NEMS. The radiative properties, such as reflectance, transmittance and emittance of multilayer structures largely depend on the direction and wavelength of incident radiation as well as wafer temperature. They are also affected by thin-film coatings and surface roughness [1].

The studied examples using silicon wafer and either silicon dioxide or silicon nitride coating demonstrate the strong influence of coating and coating thickness on the radiative properties. This study helps gain a better understanding of the radiative properties of semitransparent wafers with different coatings and will have an impact not only on semiconductor processing but also on thin film solar cells.

Fu studied radiative properties of NIMs by using three multilayer structures with NIM layer [1]. We have interested in studying nanoscale radiative properties with silicon because silicon is the most extensively used material in MEMS/NEMS.

This Paper, predict the directional, spectral and temperature dependence of the radiative properties for the

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multilayer structures consisting of silicon and related materials such as silicon dioxide and silicon nitride and compare the results of coherent formulation with incoherent formulation.

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

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

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]. Consequently, the radiative properties of the silicon wafer with thin-film coatings in the semitransparent region can be expressed as [4].

$$r = r_{ta} + \frac{t_i^2 t_t^2 r_{bs}}{1 - t_i^2 r_{ts} r_{bs}} \tag{2}$$

$$t = \frac{t_i t_t t_b}{1 - t_i^2 r_{ts} r_{bs}} \tag{3}$$

$$e = 1 - r - t \tag{4}$$

Optical Constants: 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 [5]. Li [6] developed a functional relation, for the refractive index of silicon that covers the wavelength region between 1.2 µm and 14 µm. 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 optical constants of silicon dioxide and silicon nitride are mainly based on the data collected in Palik [7].

RESULTS

Consider the case in which the silicon wafer is coated with 300 nm silicon dioxide layer on single side and both sides. The thickness of silicon wafer is 700µm and the temperature of silicon wafer with thin-film coatings are 25°C and 500°C. The Electromagnetic waves are incident at 2 = 0°. The considered wavelength range is 1µm < 8 < 7µm. Figures 1 and 2 compare calculated reflectance and transmittance with the results of reference 8. The calculated results are seen to be generally in accord with results of reference [8].

Now consider the case in which the silicon wafer is coated with a silicon dioxide layer on both sides. The thickness of silicon wafer is 500µm and the temperature of silicon wafer with thin-film coatings is 25°C and the Electromagnetic waves are incident at 2 = 0°. The considered wavelength range is 0.5µm < 8 < 2µm. The wavelengths 0.5µm < 8 < 7µm use as visible range and 0.7µm < 8 < 2µm. as near infrared range.

Oloomi *et al.* showed for lightly doped silicon that silicon dioxide coating has higher reflectance than silicon nitride coating for visible wavelengths. In visible wavelengths the reflectance increases as the temperature increases, because of decreasing emittance but in infrared wavelengths the reflectance and transmittance decrease as the temperature increases [9, 10].

Figure 3: Shows the spectral reflectance of silicon wafer coated with 200 nm silicon dioxide films on both sides. The oscillation in the reflectance in coherent formulation is due to interference in the silicon dioxide coating. This behavior is not shown in the incoherent formulation. Radiative properties are complex function of wavelength.

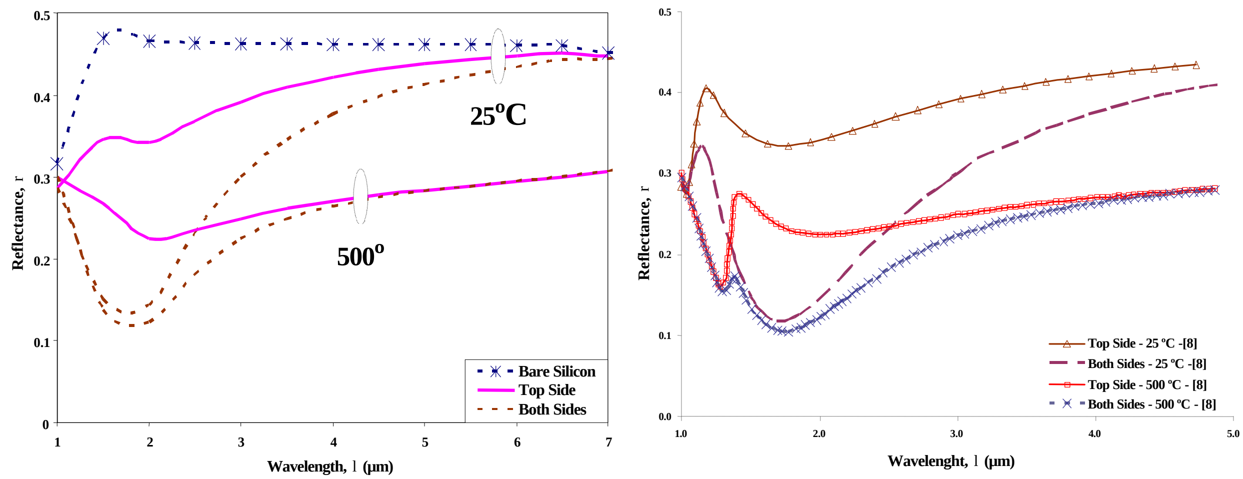

Fig. 1: A comparison of the calculated reflectance (Left side) with results of [8] (Right side)

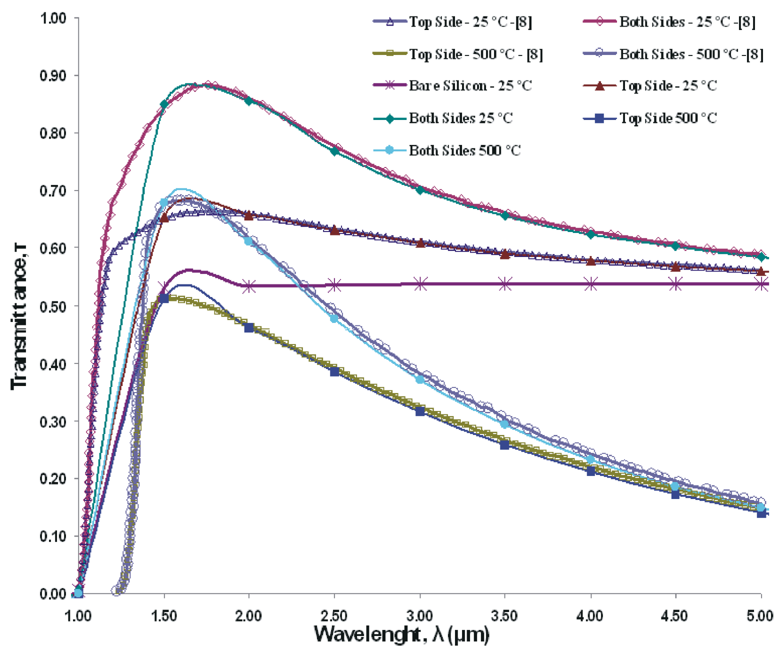

Fig. 2: A comparison of the calculated transmittance with results of [8]

Figure 4 shows the spectral transmittance of the silicon wafer with 800 nm silicon dioxide film on both sides. Results showed that transmittance for wavelength less than 1μm is negligible. The oscillation in the transmittance is due to interference in the silicon dioxide coating. The free spectral range is determined by $\Delta\lambda/\lambda^2 = (2n_f d_f)^{-1}$, where $\Delta\lambda$ is the separation between adjacent interference maxima and n_f and d_f are the refractive index and thickness of the thin film. The spectral separation $\Delta\lambda$ increases toward longer wavelengths. As the film thickness increases, the free spectral range decreases, resulting in more oscillations with the 800 nm silicon dioxide film. Therfore oscillations increased toward longer wavelengths. Figure 5 shows the spectral emittance of silicon wafer coated with 400nm silicon dioxide film on both sides. Emittance increases with increasing in wavelength for 0.6μm < λ < 0.8μm, but for 0.5μm < λ < 0.6μm and 0.8μm < λ < 1.2μm, emittance decrease with increasing in wavelength.

The average reflectance and emittance of silicon wafer coated with silicon dioxide film on both sides, at room temperatures and normal incidence in visible wavelengths as function of thickness are showed in Tables 1 and 2.

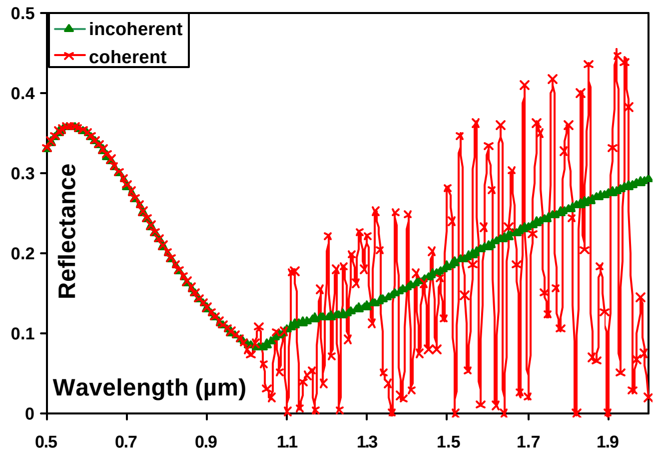

Fig. 3: Spectral Reflectance of silicon wafer coated with 200 nm silicon dioxide films on both sides, at room temperatures

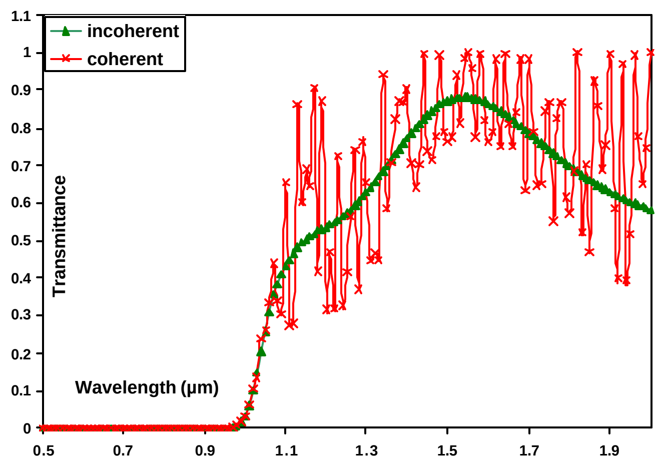

Fig. 4: Spectral Transmittance of silicon wafer coated with 800 nm silicon dioxide films on both sides, at room temperatures

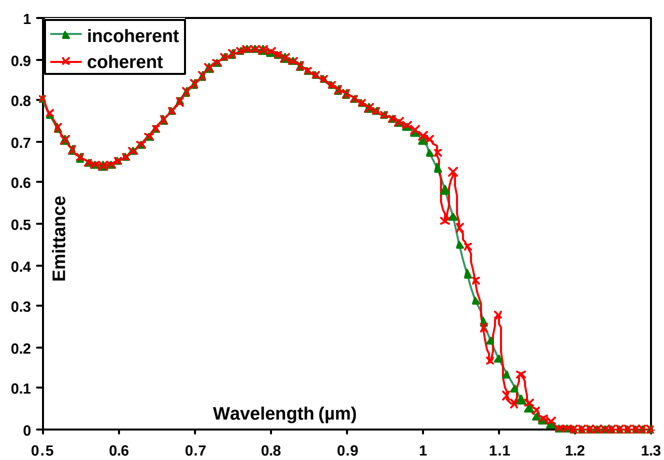

Fig. 5: Spectral Emittance of silicon wafer coated with 400 nm silicon dioxide films on both sides, at room temperatures

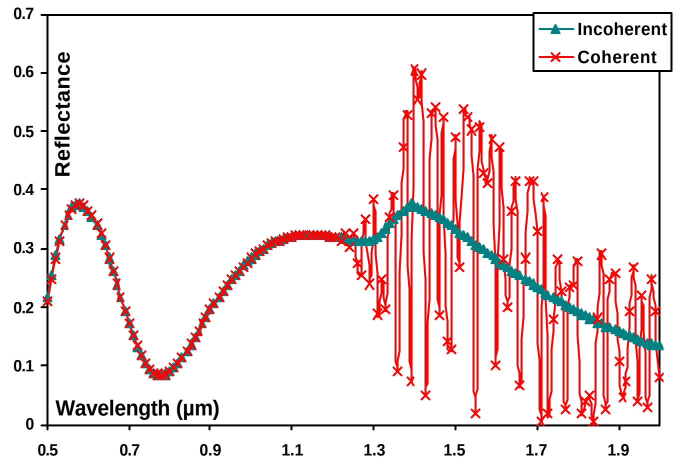

Fig. 6: Spectral Reflectance of silicon wafer coated with 400 nm silicon dioxide film on both sides at 500°C.

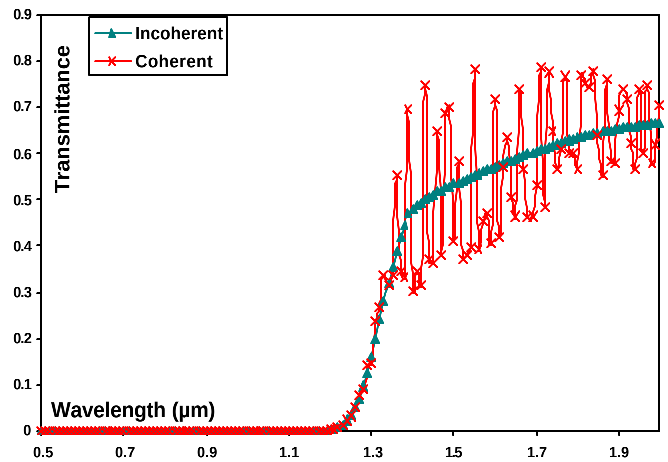

Fig. 7: Spectral Transmittance of silicon wafer coated with 400 nm silicon dioxide film on both sides at 500°C.

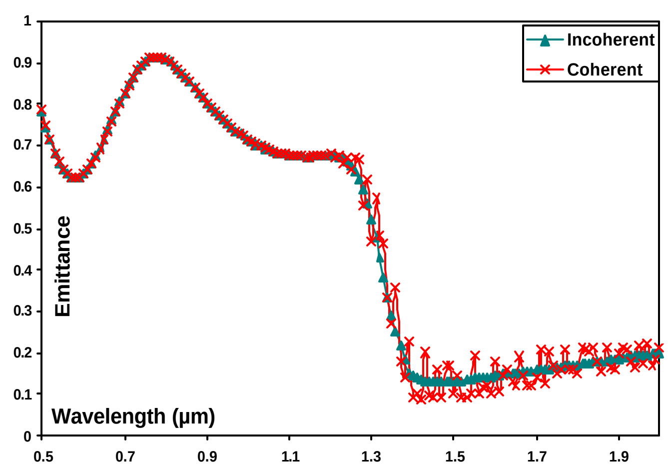

Fig. 8: Spectral Emittance of silicon wafer coated with 400 nm silicon dioxide film on both sides at 500°C.

Table 1: Average Reflectance of silicon wafer coated with silicon dioxide film on both sides, at room temperatures in Visible Wavelengths

Silicon Dioxide Thickness/ Formulation	Coherent Formulation	Incoherent Formulation
200 nm	0.336154	0.336199
400 nm	0.282481	0.282565
600 nm	0.223792	0.223833
800 nm	0.203667	0.203632

Table 2: Average Emittance of silicon wafer coated with silicon dioxide film on both sides, at room temperatures in Visible Wavelengths

Silicon Dioxide Thickness/ Formulation	Coherent formulation	Incoherent Formulation
200 nm	0.663846	0.663801
400 nm	0.717519	0.717435
600 nm	0.776208	0.776167
800 nm	0.796333	0.796368

Table 3: Average Reflectance of silicon wafer coated with silicon dioxide film on both sides with normal incidence in Near Infrared Wavelengths

Wafer Temperature/ Formulation	Coherent Formulation	Incoherent Formulation
25°C	0.295619	0.284717
500°C	0.251555	0.248525
1000°C	0.216841	0.216776

Table 4: Average Emittance of silicon wafer coated with silicon dioxide film on both sides with normal incidence in Near Infrared Wavelengths

Wafer Temperature/ Formulation	Coherent formulation	Incoherent Formulation
25°C	0.237899	0.235362
500°C	0.446625	0.445635
1000°C	0.783159	0.783224

Table 5: Average Reflectance of silicon wafer coated with silicon dioxide film on both sides with normal incidence in Visible Wavelengths

Thin Film Coating/ Formulation	Coherent Formulation	Incoherent Formulation
Silicon Dioxide Coating	0.282481	0.282565
Silicon Nitride Coating	0.180527	0.180560

Table 6: Average Emittance of silicon wafer coated with silicon dioxide film on both sides with normal incidence in Visible Wavelengths

Thin Film Coating/ Formulation	Coherent formulation	Incoherent Formulation
Silicon Dioxide Coating	0.717519	0.717435
Silicon Nitride Coating	0.819473	0.819440

For visible wavelengths, the reflectance decreases 60% as the coating thickness increases from 200 nm to 800 nm and the emittance increases 20% as the coating thickness increases from 200 nm to 800 nm. In these wavelengths, transmittance is negligible. Average radiative properties of wafer are approximated equal for both formulations, but oscillation in the radiative properties in coherent formulation is due to interference in the coating are showed.

The spectral reflectance, transmittance and emittance of silicon wafer coated with 400 nm silicon dioxide film on both sides at 500°C are showed in Figures 6 to 8.

The average reflectance and emittance of silicon wafer coated with 400 nm silicon dioxide film on both sides with normal incidence in near infrared wavelengths as function of temperature are showed in Tables 3 and 4. In visible wavelengths the reflectance increases as the temperature increases, because of decreasing emittance but in infrared wavelengths the reflectance and transmittance decrease as the temperature increases. The increase in temperature causes both the reflectance and transmittance to decrease due to the increase in the absorption coefficient (Table 3). Therefore, the emittance at 500°C is greater than that at room temperature (Table 4). The interference effect is enhanced with double-side coatings. The result is an increase in the transmittance and a reduction in the reflectance at certain wavelengths (Figures 1 and 2). The emittance changes slightly between the case of single-side and double-side coating (not shown in Figures 1 and 2).

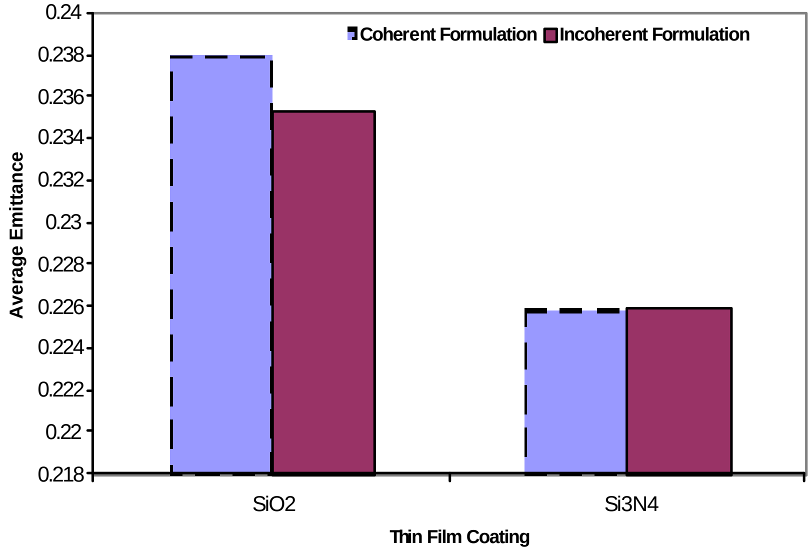

Fig. 9: Average Emittance of silicon wafer coated with thin films (silicon dioxide and silicon nitride) on both sides (400 nm thickness) for near infrared wavelengths, at room temperatures and normal incidence

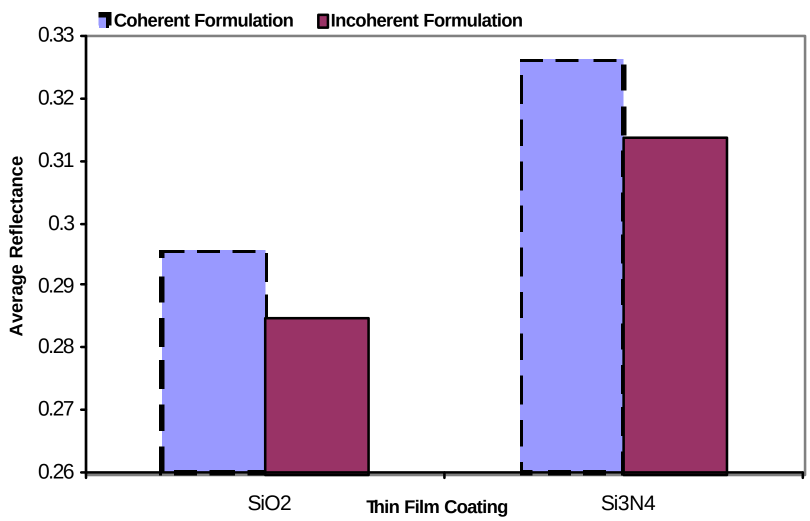

Fig. 10: Average Reflectance of silicon wafer coated with thin films (silicon dioxide and silicon nitride) on both sides (400 nm thickness) for near infrared wavelengths, at room temperatures and normal incidence

The average reflectance and emittance of silicon wafer coated with 400 nm different thin film coatings on both sides with normal incidence in visible wavelengths are showed in Tables 5 and 6. The average emittance and reflectance of silicon wafer coated with 400 nm thin film coatings on both sides in near infrared wavelengths at room temperature and normal incidence are showed in Figures 9 to 10.

When the silicon substrate is coated with a SiO_2 or Si_3N_4 film, which serves as an antireflection coating, the reflectance oscillates from a minimum to a maximum, equal to the reflectance of silicon without coating (Figure 6).

Silicon dioxide coating has higher emittance than silicon nitride coating for 0.7μm < 8 < 0.9μm, but for 0.5μm < 8 < 0.7μm and 0.9μm < 8 < 1μm silicon nitride coating has higher emittance than silicon oxide coating. Silicon dioxide coating has higher reflectance than silicon nitride coating for visible wavelengths [9, 10].

In near infrared wavelengths, silicon nitride coating has higher average reflectance than silicon oxide coating and silicon dioxide coating has higher average emittance than silicon nitride coating (Figures 9, 10). In visible wavelengths, silicon nitride coating has higher average emittance than silicon oxide coating and silicon dioxide coating has higher average reflectance than silicon nitride coating (Tables 5, 6). Therefore coatings act as wavelength selective emitters for radiative energy conversion and thermal radiation detection. Interferences in the substrate are generally not observable in Incoherent Formulation (Figures 4 to 8). This is the major difference between coherent and incoherent Formulation.

CONCLUSIONS

We have analyzed and calculated the spectral, directional and temperature dependency of radiative properties of a three layers material using transfer-matrix method. In the present work empirical expressions are carefully selected for calculating the optical constants of materials. Results are compared with the results of reference 8. The calculated results are seen to be generally in accord with results of reference [8].

Results Showed That:

- The effect of wave interference can be understood by plotting the spectral properties such as reflectance or transmittance of a thin dielectric film versus the film thickness and analyzing the oscillations of properties due to constructive and destructive interferences.
- As the film thickness increases, the free spectral range decreases, resulting in more oscillations with the 800-nm silicon dioxide film.
- Results showed that for lower wavelengths, more emittance occurs in thicker coatings.
- The layer thicknesses need to be optimized to achieve maximum transmittance for the given materials.
- Maximum transmittance also depends on the type of coatings and their temperatures.
- In visible wavelengths the reflectance increases as the temperature increases, because of decreasing emittance.
- In infrared wavelengths the reflectance and transmittance decrease as the temperature increases, because of increasing emittance.
- The interference effect is enhanced with double-side coatings. The result is an increase in the transmittance and a reduction in the reflectance at certain wavelengths.
- When the silicon substrate is coated with a SiO_2 or Si_3N_4 film, which serves as an antireflection coating, the reflectance oscillates from a minimum to a maximum, equal to the reflectance of silicon without coating.
- In visible wavelengths, silicon nitride coating has higher average emittance than silicon oxide coating and silicon dioxide coating has higher average reflectance than silicon nitride coating.
- Interferences in the substrate are generally not observable in incoherent Formulation.
- Coatings act as wavelength selective emitters for radiative energy conversion and thermal radiation detection.

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