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Nanoscale Radiative Properties of Thin Films

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Abstract: A great number of the optical components and semiconductors are being covered with thin films, so study of the surfaces which covered by thin films are very important. This work uses transfer-matrix method for calculating the radiative properties. Results showed that maximum transmittance depends on the type of materials coatings and its temperature. The reflectance decreases as the temperature increases, because of increasing emittance. The coatings act as wavelength selective emitters for radiative energy conversion and thermal radiation detection. When silicon dioxide thin film coating thickness increases to 300 nm then reflectance of multilayer decreases from 0.4553 to 0.0443. The layer thicknesses need to be optimized to achieve maximum transmittance for the given materials.

Key words: Thickness · Temperature · Thin Film · Nanoscale · Emittance · Reflectance · Transmittance

INTRODUCTION

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 [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]. Silicon is the semiconductor that plays a vital role in integrated circuits and MEMS/NEMS. This work interested in silicon, because of its various applications.

During the past two decades, there have been tremendous developments in near-field imaging and local probing techniques. Examples are the Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), Near-field Scanning Optical Microscopy (NSOM), Photon Scanning Tunneling Microscopy (PSTM) and Scanning Thermal Microscopy (SThM).

Spectral and directional control of thermal radiation is a challenging yet important task for a number of applications, such as thermophotovoltaic (TPV) energy conversion, solar energy utilization, space thermal management and high-efficiency incandescent lamps.

Temperature measurements and control are critically important for continuous improvement of RTP [2, 3]. Since the heating source is at a much higher temperature than that of the silicon wafer, radiative energy exchange is the dominant mode of heat transfer. Hence, understanding the radiative properties of silicon and other relevant materials is essential for the analysis of the thermal transport processes. Furthermore, since many RTP furnaces use noncontact lightpipe thermometers, accurate determination of the wafer emittance is necessary for correlating the radiance temperature to the true wafer temperature [4, 5].

Knowledge of the radiative properties of multilayer consisting of silicon and related materials, such as silicon dioxide (SiO_2), silicon nitride (Si_3N_4) and gold (Au) with different thicknesses is required for many microsystem applications. [6]. In visible wavelengths the reflectance increases as the temperature increases, because of decreasing emittance. 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 [7].

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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 [8]. Interferences in the substrate are generally not observable in the incoherent formulation. This is the major difference between coherent and incoherent formulations [9]. 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.

For lightly doped silicon, silicon dioxide coating has higher reflectance than silicon nitride coating for visible wavelengths. In visible wavelengths the reflectance increases as the temperature increases due to decreasing emittance; but in infrared wavelengths, the reflectance and transmittance decrease as the temperature increases [9].

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.

Modeling the Radiative Properties of Multilayers

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 become important to correctly predict the radiative properties of multilayer structure of thin films. The transfer-matrix method provides a convenient way to calculate the radiative properties of multilayer structures of thin films (Figure 1).

By assuming that the electric field in the jth medium is a summation of forward and backward waves in the z-direction, the electric field in each layer can be expressed by

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

Where A_j and B_j are the amplitudes of forward and backward waves in the jth layer. Detailed descriptions of how to solve for A_j and B_j is given in [1]. Consequently, the radiative properties of the N-layer system are given by

$$\rho = \frac{B_1 B_1^*}{A_1^2}, \tau = \frac{\mathrm{Re}\left(\tilde{n}_N \cos\tilde{\theta}_N\right)}{n_1 \cos\theta_1} \frac{A_N A_N^*}{A_1^2}, \varepsilon = 1 - \rho - \tau \quad (2)$$

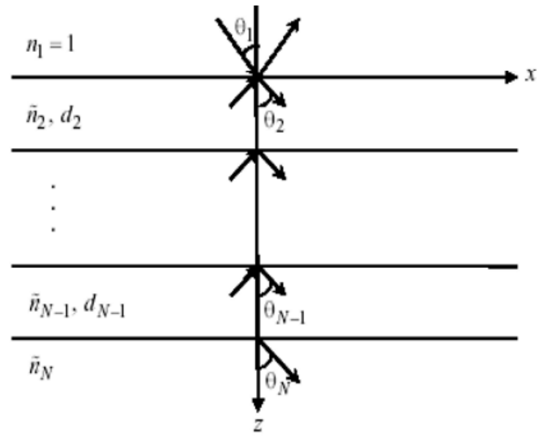

Fig. 1: The geometry for calculating the radiative properties of a multilayer structure

Optical Constants: The optical constants, including the refractive index (n) and the extinction coefficient (κ), of a material are complicated functions of the wavelength and temperature.

The Refractive Index of Silicon: Jellison and Modine [10] measured the ratio of the Fresnel reflection coefficients of silicon wafers in both polarization states with a two-channel spectroscopic ellipsometer in the temperature range from 25°C to 490 °C. From the measurement results, they extracted the refractive index and extinction coefficient using the least-squares Levenberg-Marquardt fitting.

The Jellison and Modine (J-M) expression of the refractive index for wavelength between 0.4 µm and 0.84 µm is given by

$$n_{JM}(\lambda, T) = n_0(\lambda) + \beta(\lambda)T \quad (3)$$

$$n_0 = \sqrt{4.565 + \frac{97.3}{3.648^2 - (1.24/\lambda)^2}} \quad (4)$$

$$\beta(\lambda) = -1.864 \times 10^{-4} + \frac{5.394 \times 10^{-3}}{3.648^2 - (1.24/\lambda)^2} \quad (5)$$

Where $\lambda[\mu m]$ is the wavelength in vacuum and T [°C] is the temperature.

Li [11] extensively reviewed the refractive index of silicon. By carefully analyzing published experimental data, he developed a functional relation, based on the modified Sellmeier type dispersion relation, for the refractive index of silicon that covers the wavelength region between 1.2 µm and 14 µm and the temperature range up to 480°C.

$$n_L(\lambda,T) = \sqrt{\varepsilon_r(T) + \frac{g(T)\eta(T)}{\lambda^2}} \tag{6}$$

$$\varepsilon_r(T) = 11.631 + 1.0268\times10^{-3}T + 1.0384\times10^{-6}T^2 - 8.1347\times10^{-10}T^3 \tag{7}$$

$$g(T) = 1.0204 + 4.8011\times10^{-4}T + 7.3835\times10^{-8}T^2 \tag{8}$$

$$\eta(T) = \exp(1.786\times10^{-4} - 8.526\times10^{-6}T - 4.685\times10^{-9}T^2 + 1.363\times10^{-12}T^3) \tag{9}$$

To calculate the refractive index of silicon, in this study the J-M expression is used in the wavelength region from 0.5 µm to 0.84 µm and Li's expression at wavelengths above 1.2 µm. In the wavelength range between 0.84 µm and 1.2 µm, we use a weighted average based on the extrapolation of the two expressions.

The Extinction Coefficient of Silicon: The extinction coefficient (κ) and absorption coefficient (α) are related by $\alpha = 4\pi k / \lambda$.

The absorption coefficient of silicon depends on the absorption processes, such as interband transition, intraband transition and free-carrier absorption. When the photon energy is higher than the band gap energy of silicon, electrons in the valance band can be excited to the conduction band, resulting in a large absorption coefficient.

The J-M expression of the extinction coefficient, covering the wavelength range from 0.4 µm to 0.84 µm, is given as [10]:

$$k_{JM}(\lambda,T) = k_0(\lambda)\exp\left[\frac{T}{369.9 - \exp(-12.92 + 6.831/\lambda)}\right]$$

$$k_0(\lambda) = -0.0805 + \exp\left[-3.1893 + \frac{7.946}{3.648^2 - (1.24/\lambda)^2}\right]$$

The absorption coefficient can be deduced from the extinction coefficient.

In the longer wavelength region, Timans [12] measured the emission spectra of several silicon wafers and deduced the absorption coefficient in the wavelength region from 1.1 µm to 1.6 µm, in the temperature range between 330°C and 800°C. He suggested that the absorption coefficient can be expressed as a summation of the band gap absorption and free-carrier absorption as following:

$$\alpha(\lambda,T) = \alpha_{BG}(\lambda,T) + \alpha_{FC}(\lambda,T) \tag{10}$$

The expression for the band gap absorption can be found in the work by MacFalane *et al*. [13] and is given by

$$\alpha_{BG}(\lambda,T) = \sum_{i=1}^{4}\alpha_{a,i}(\lambda,T) + \sum_{i=1}^{2}\alpha_{e,i}(\lambda,T) \tag{11}$$

Notice that silicon is an indirect-gap semiconductor and the absorption process is accompanied by either the absorption of a phonon, denoted by $\alpha_{\alpha,i}(\lambda,T)$ or the emission of a phonon, denoted by $\alpha_{e,i}(\lambda,T)$. Detailed expressions for $\alpha_{\alpha,i}(\lambda,T)$ and $\alpha_{e,i}(\lambda,T)$ can be found in Timans [12, 14].

For the free-carrier absorption, Sturm and Reaves [15] suggested an expression based on their measurement of the transmission of the wafer at 1.30 µm and 1.55 µm and in the temperature range of 500°C to 800°C. The Sturm and Reaves (S-R) expression is

$$\alpha_{FC} = N_e A_e + N_h A_h \tag{12}$$

Where N_e and N_h are electron and hole concentrations and A_e and A_h are electron and hole absorption cross sections, respectively. The Vandenabeele and Maex (V-M) expression is given by [16]

$$\alpha_{FC}(\lambda,T) = 4.15\times10^{-5}\lambda^{151} (T+273.15)^{2.95}\times\exp\left(\frac{-700}{T+273.15}\right) \tag{13}$$

Here again, T is in °C. Rogne *et al*. [17] demonstrated that the absorption coefficient calculated from the V-M expression agrees well with experimental data in the wavelength region between 1.0 µm and 9.0 µm at elevated temperatures.

In the wavelength region between 6.0 µm and 25.0 µm, lattice vibrations causes an additional absorption. Since the effect of lattice absorption is negligible in most RTP applications compared to the absorption by free carriers, it is assumed to be independent of the temperature and dopant concentration. The extinction coefficient for lightly doped silicon due to the lattice absorption is simply obtained from the tabulated extinction coefficient values given in Ref. [18] at room temperature.

The optical constants of silicon dioxide and silicon nitride are mainly based on the data collected in Palik's handbook [19, 20].

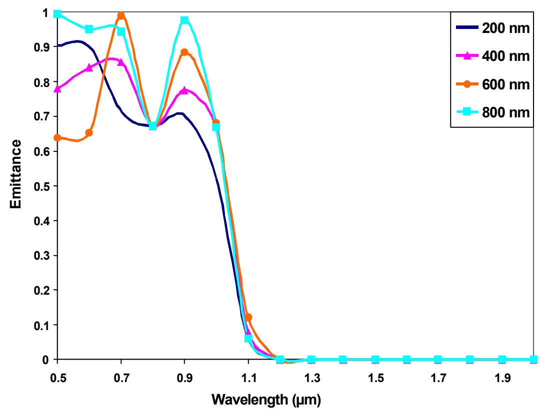

Fig. 2: Spectral Emittance of silicon wafer coated with silicon nitride film with different thicknesses (200 nm, 400nm, 600nm, 800nm) on both sides, at room Temperatures and normal incidence

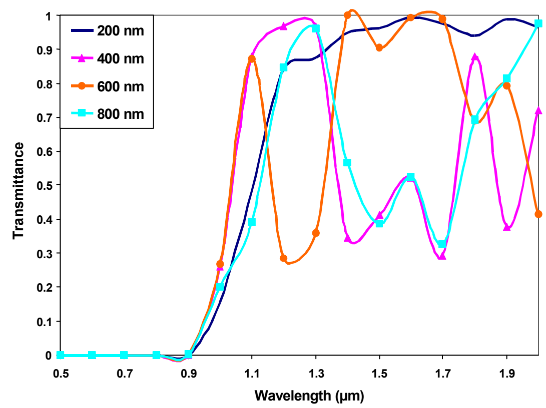

Fig. 3: Spectral Transmittance of silicon wafer coated with silicon nitride film with different thicknesses (200 nm, 400nm, 600nm, 800nm) on both sides, at room Temperatures and normal incidence

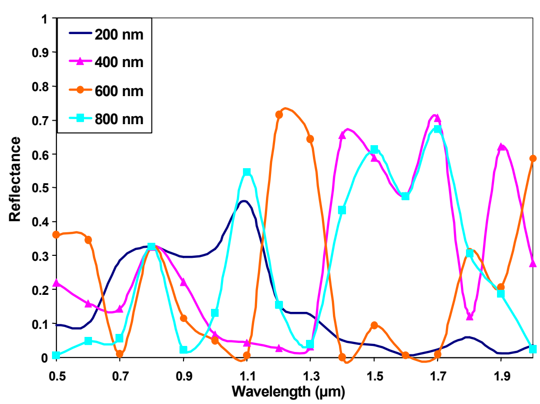

Fig. 4: Spectral Reflectance of silicon wafer coated with silicon nitride film with different thicknesses (200 nm, 400nm, 600nm, 800nm) on both sides, at room Temperatures and normal incidence

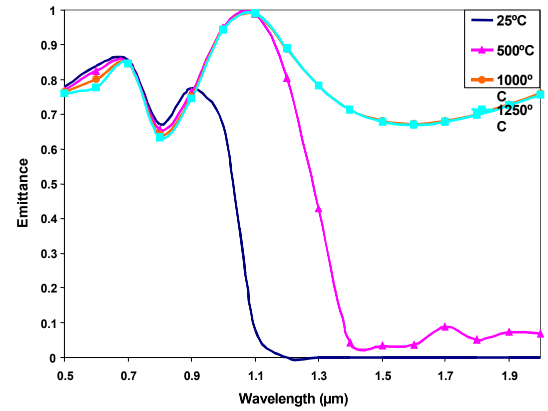

Fig. 5: Spectral Emittance of silicon wafer coated with silicon nitride film (400 nm thickness) on both sides at different Temperatures (25°C, 500°C, 1000°C, 1250°C)

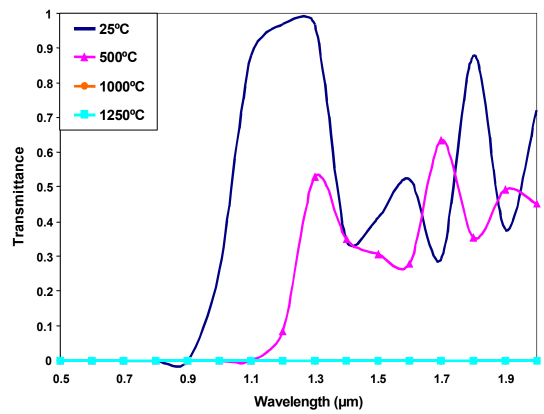

Fig. 6: Spectral Transmittance of silicon wafer coated with silicon nitride film (400 nm thickness) on both sides at different Temperatures (25°C, 500°C, 1000°C, 1250°C).

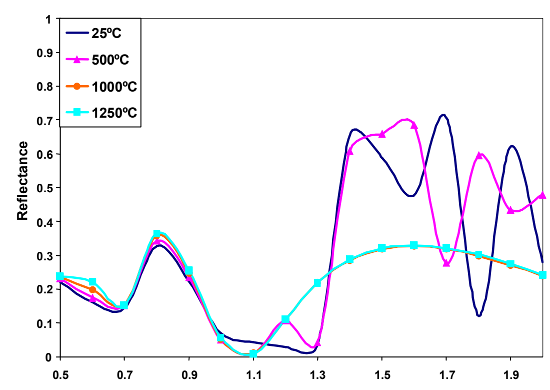

Fig. 7: Spectral Reflectance of silicon wafer coated with silicon nitride film (400 nm thickness) on both sides at different Temperatures (25°C, 500°C, 1000°C, 1250°C).

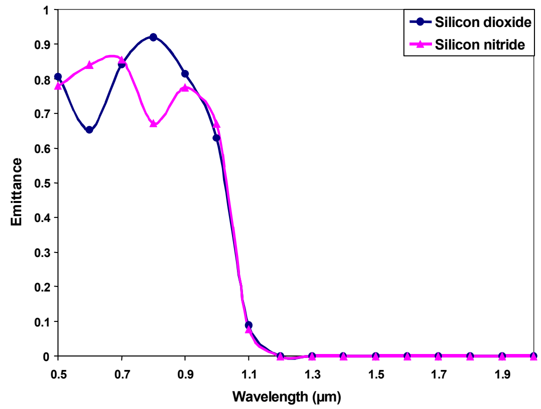

Fig. 8: Spectral Emittance of silicon wafer coated with different materials (silicon dioxide and silicon nitride) on both sides (400 nm thickness), at room Temperatures and normal incidence.

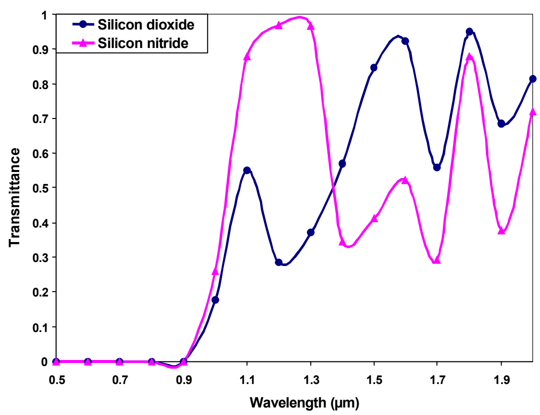

Fig. 9: Spectral Transmittance of silicon wafer coated with different materials on both sides (400 nm thickness), at room Temperatures and normal incidence.

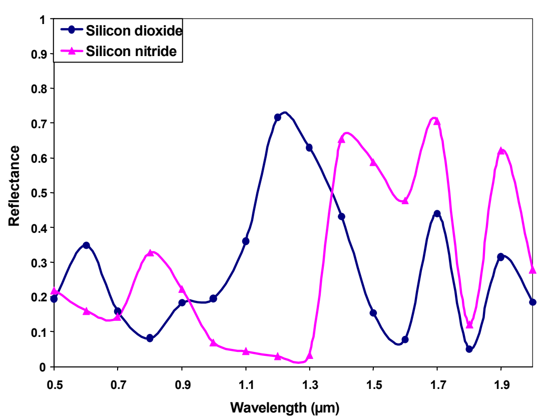

Fig. 10: Spectral Reflectance of silicon wafer coated with different materials on both sides (400 nm thickness), at room Temperatures and normal incidence.

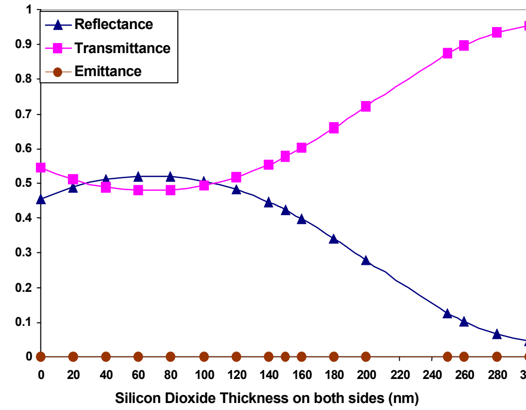

Fig. 11: Radiative Properties of silicon wafer coated with silicon dioxide thin film on both sides with different thicknesses at room Temperature and normal incidence.

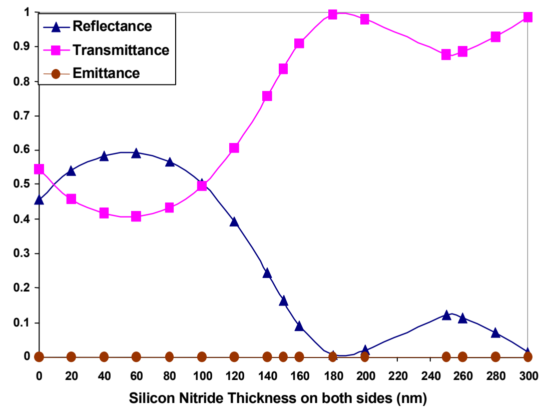

Fig. 12: Radiative Properties of silicon wafer coated with silicon nitride thin film on both sides with different thicknesses at room Temperature and normal incidence.

RESULTS

Consider the case in which the silicon wafer is coated with a silicon nitride layer on both sides. The thickness of silicon wafer is $200\mu m$ and the temperature of silicon wafer with thin-film coatings is 25°C and the EM waves are incident at $\theta = 0°$. The considered wavelength range is $0.5\mu m < \lambda < 2.0\mu m$. Some results of this study are shown below in figures 2 to 10.

CONCLUSIONS

This work analyzed and calculated the spectral, directional and temperature dependency of radiative properties of a three layers material using transfer-matrix method.

Results Showed That:

- The layer thicknesses need to be optimized to achieve maximum transmittance for the given materials.
- Maximum transmittance also depends on the type of materials coatings and its temperature.
- 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.
- For lower wavelengths, more emittance occurs in thicker coatings.
- The reflectance decreases as the temperature increases, because of increasing emittance.
- Silicon dioxide coating has higher emittance than silicon nitride coating for $0.7\mu m < \lambda < 0.9\mu m$, but for $0.55\mu m < \lambda < 0.7\mu m$ and $0.9\mu m < \lambda < 1.0\mu m$ silicon nitride coating has higher emittance than silicon oxide coating.
- The coatings act as wavelength selective emitters for radiative energy conversion and thermal radiation detection.
- Increasing thickness of thin film coating up to 100 nm has not any effect on the radiative properties of multilayer for both coatings. If thin film thickness increases greater than 100 nm then transmittance increases and reflectance decreases rapidly.
- When silicon nitride thin film coating thickness increases to 300 nm then reflectance of multilayer decreases about 97%.
- When silicon dioxide thin film coating thickness increases to 300 nm then reflectance of multilayer decreases from 0.4553 to 0.0443.
- Industrial requirements are supported by selecting coating's material and thickness.

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