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Effects of Dopant Concentrations on Radiative Properties of Nanoscale Multilayer with Coherent Formulation for Visible Wavelengths

S. A. A. Oloomi , M. Omidpanah

Abstract**—**Semiconductor materials with coatings have a wide range of applications in MEMS and NEMS. This work uses transfer-matrix method for calculating the radiative properties. Dopped silicon is used and the coherent formulation is applied. The Drude model for the optical constants of doped silicon is employed. Results showed that for the visible wavelengths, more emittance occurs in greater concentrations and the reflectance decreases as the concentration increases. In these wavelengths, transmittance is negligible. Donars and acceptors act similar in visible wavelengths. 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. But this effect has not been shown at visible wavelengths. At room temperature, the scattering process is dominated by lattice scattering for lightly doped silicon, and the impurity scattering becomes important for heavily doped silicon when the dopant concentration exceeds $10^{18}\ cm^{-3}$.

Keywords**—**Dopant Concentrations-Radiative Properties-Nanoscale Multilayer-Coherent Formulation-Visible Wavelengths

I. INTRODUCTION

UNDERSTANDING the radiative properties of semiconductors is essential for the advancement of manufacturing technology, such as rapid thermal processing [1]. Because the major heating source in rapid thermal processing is lamp radiation, knowledge of radiative properties is important for temperature control during the process. Silicon is semiconductor that plays a vital role in integrated circuits and MEMS/NEMS [2]. Semitransparent crystalline silicon solar cells can improve the efficiency of solar power generation [3]. 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 [4].

For lightly dopped 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. [2, 5]. 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 [6-7].

S.A.A.Oloomi is with Department of Mechanical Engineering, Yazd Branch, Islamic Azad University, Yazd, Iran , Tel: +98-9133593179, Email: AmirOloomi@iauyazd.ac.ir.

M. Omidpanah is with Department of Mechanical Engineering, Technical & Vocational University, Yazd, Iran

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 [6]. This work uses transfer-matrix method for calculating the radiative properties. Dopped silicon is used and the coherent formulation is applied. The Drude Model for the Optical Constants of Doped Silicon is employed. Phosphorus and boron are default impurities for n-type and p-type, respectively in this work.

II. MODELING

A. 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 (Fig. 1).

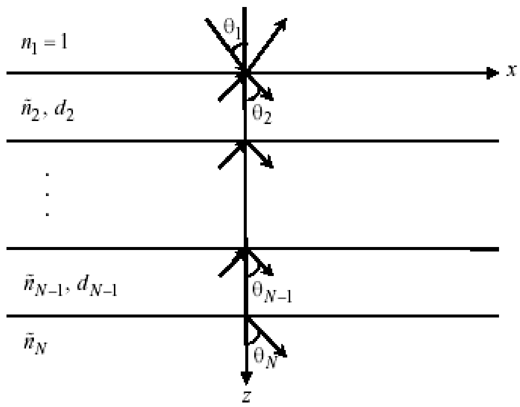

Fig. 1 The geometry for calculating the radiative properties of a multilayer structure

By 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

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

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 [8].

III. THE DRUDE MODEL FOR THE OPTICAL CONSTANTS OF DOPED SILICON

The complex dielectric function is related to the refractive index (n) and the extinction coefficient (κ) by this equation

$$\varepsilon(\omega) = (n + ik)^2 \quad (2)$$

To account for the doping effects, the Drude model is employed, and the dielectric function of both intrinsic and doped silicon is expressed as the following form [9]

$$\varepsilon(\omega) = \varepsilon_{bl} - \frac{N_e e^2 / \varepsilon_0 m_e^*}{\omega^2 + i\omega / \tau_e} - \frac{N_h e^2 / \varepsilon_0 m_h^*}{\omega^2 + i\omega / \tau_h} \quad (3)$$

Where the first term in the right (ε_{bl}) accounts for contributions by transitions across the band gap and lattice vibrations, the second term is the Drude term for transitions in the conduction band (free electrons), and the last term is the Drude term for transitions in the valence band (free holes). Here, N_e and N_h are the concentrations, m_e^* and m_h^* the effective masses, τ_e and τ_h the scattering times for free electrons and holes, respectively, and e is the electron charge.

In this work, the expression of Jellison and Modine [8] is used to calculate the refractive index n_{bl} in the wavelength region from 0.5 μm to 0.84 μm.

$$n_{bl}(\lambda, T) = n_0(\lambda) + \beta(\lambda)T \quad (4)$$

$$n_0 = \sqrt{4.565 + \frac{97.3}{3.648^2 - (1.24/\lambda)^2}} \quad (5)$$

$$\beta(\lambda) = -1.864 \times 10^{-4} + \frac{5.394 \times 10^{-3}}{3.648^2 - (1.24/\lambda)^2} \quad (6)$$

The scattering time τ_e or τ_h depends on the collisions of electrons or holes with lattice (phonons) and ionized dopant sites (impurities or defects); hence, it generally depends on the temperature and dopant concentration. The total scattering time (for the case of τ_e), which consists of the above two mechanisms, can be expressed as [9]

$$\frac{1}{\tau_e} = \frac{1}{\tau_{e-l}} + \frac{1}{\tau_{e-d}} \quad (7)$$

Where τ_{e-l} and τ_{e-d} denote the electron-lattice and electron-defect scattering time, respectively.

IV. Result

Consider the case in which the silicon wafer is coated with a silicon dioxide layer on both sides. The thickness of silicon wafer is 500 μm and the temperature of silicon wafer with thin-film coatings is 25ºC and the Electromagnetic waves are incident at $\theta = 0^\circ$. The considered wavelength range is $0.5 \mu m < \lambda < 0.7 \mu m$. Dopped silicon is used and the coherent formulation is applied. The thickness of SiO_2 is 400 nm. The Drude Model for the Optical Constants of Doped Silicon is employed. The optical constants of silicon dioxide and silicon nitride are mainly based on the data collected in Palik's handbook [10-11]. Phosphorus acts as donar (n-type) and born acts as acceptor (p-type) for dopped silicon. Increasing number of thin film layers lead to more complexity and dependency on wavelength regard to wavelength interferences [12]. At infrared wavelengths, lower reflectance occurs at higher concentrations and emittance increases with increasing concentration [13]. 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 [14].

Some results of this study are shown below in figures 2 to 10.

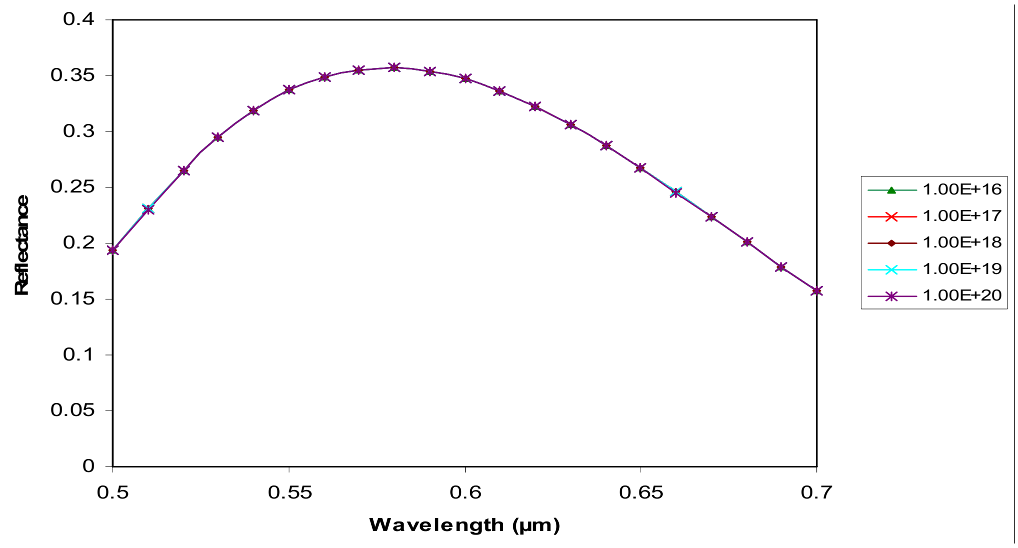

Fig. 2 Spectral Reflectance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (n-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

V. Conclusions

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 [5-6]. 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 [6].

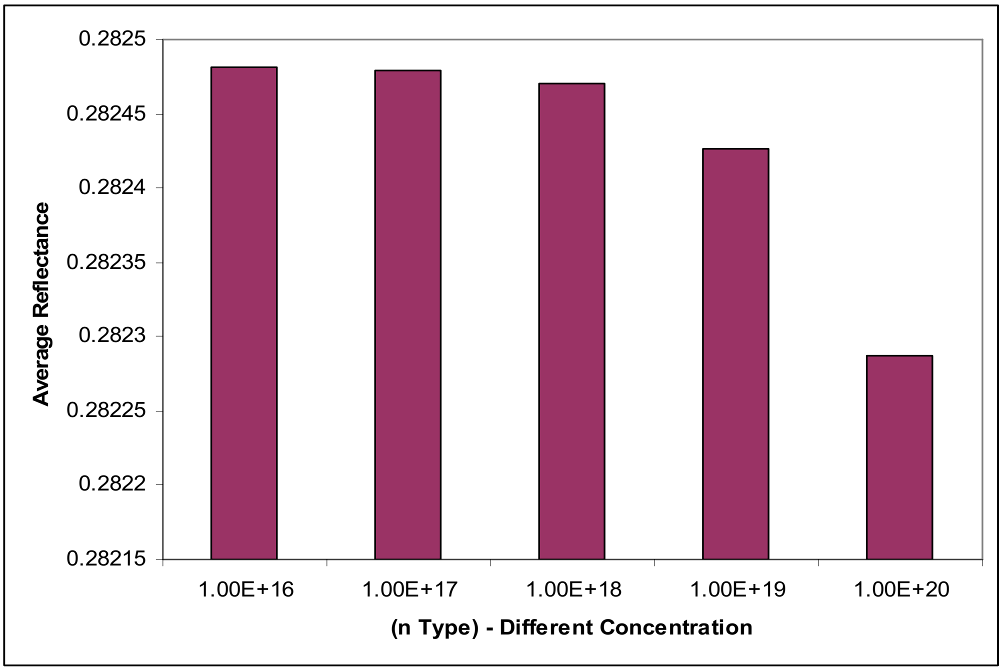

Fig. 3 Average Reflectance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (n-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

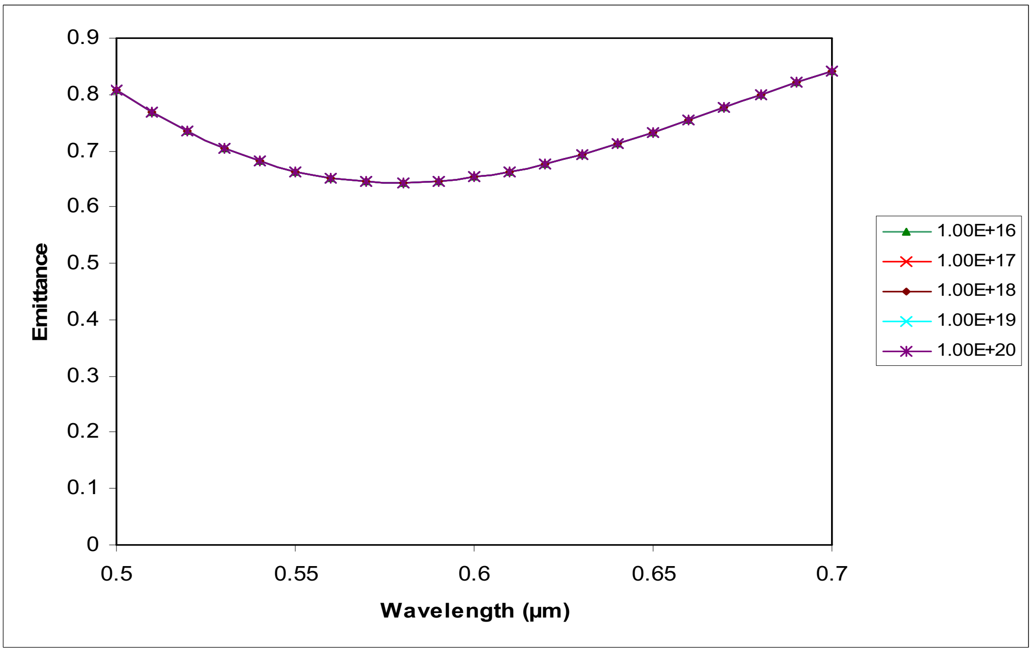

Fig. 4 Spectral Emittance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (n-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

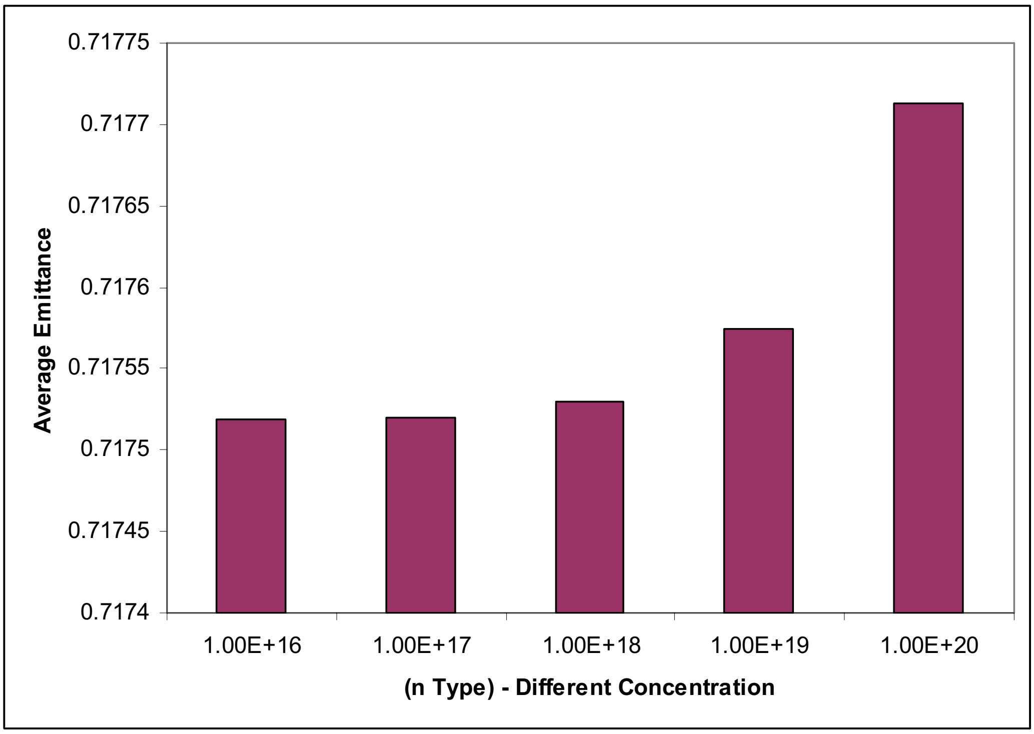

Fig. 5 Average Emittance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (n-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

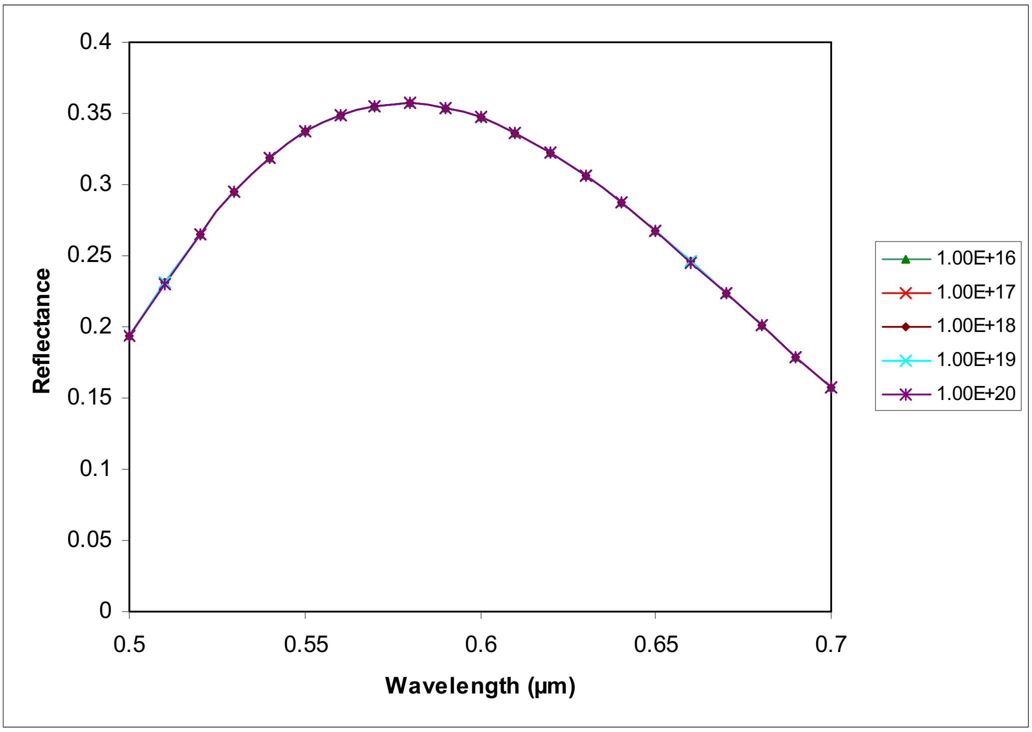

Fig. 6 Spectral Reflectance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (p-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

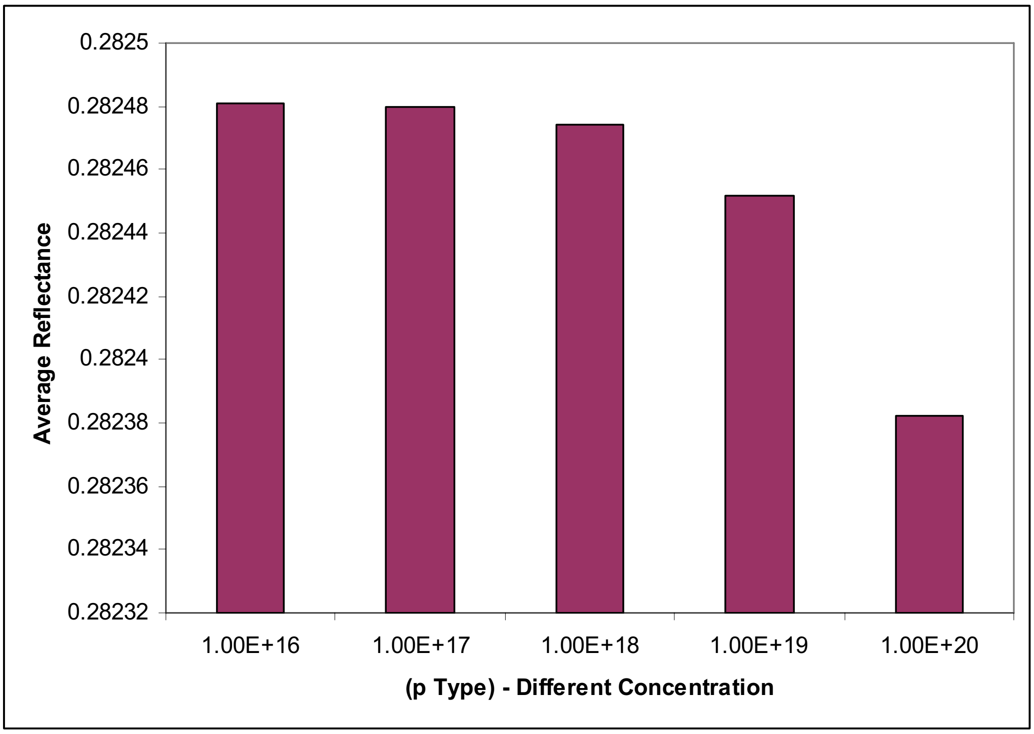

Fig. 7 Average Reflectance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (p-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

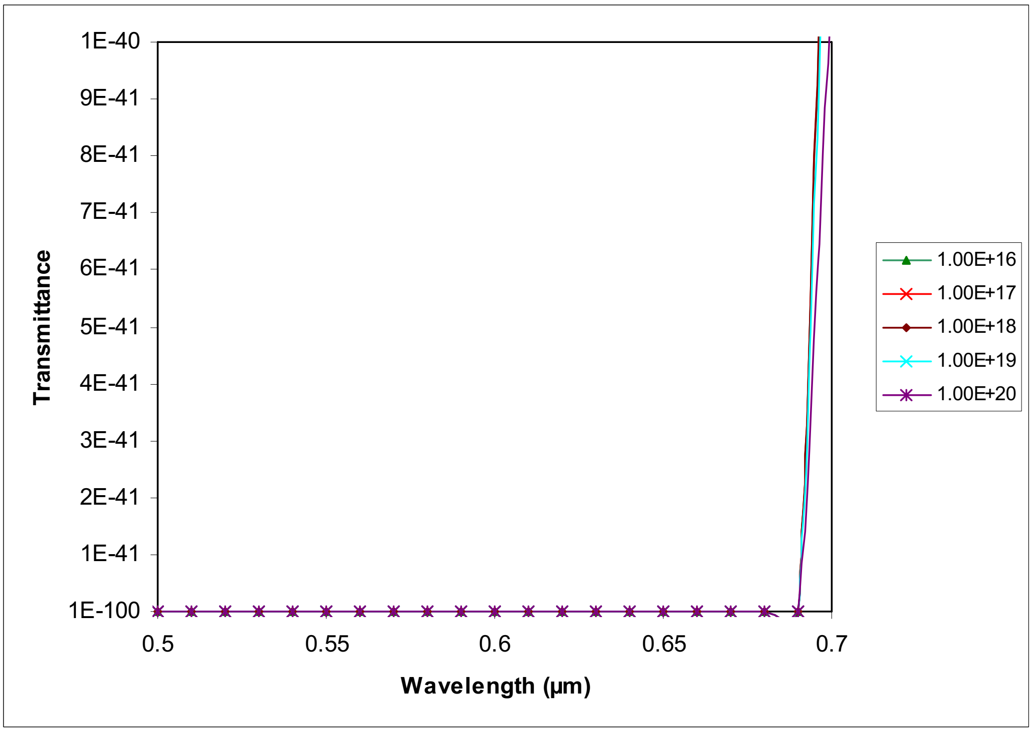

Fig. 8 Spectral Transmittance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (p-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

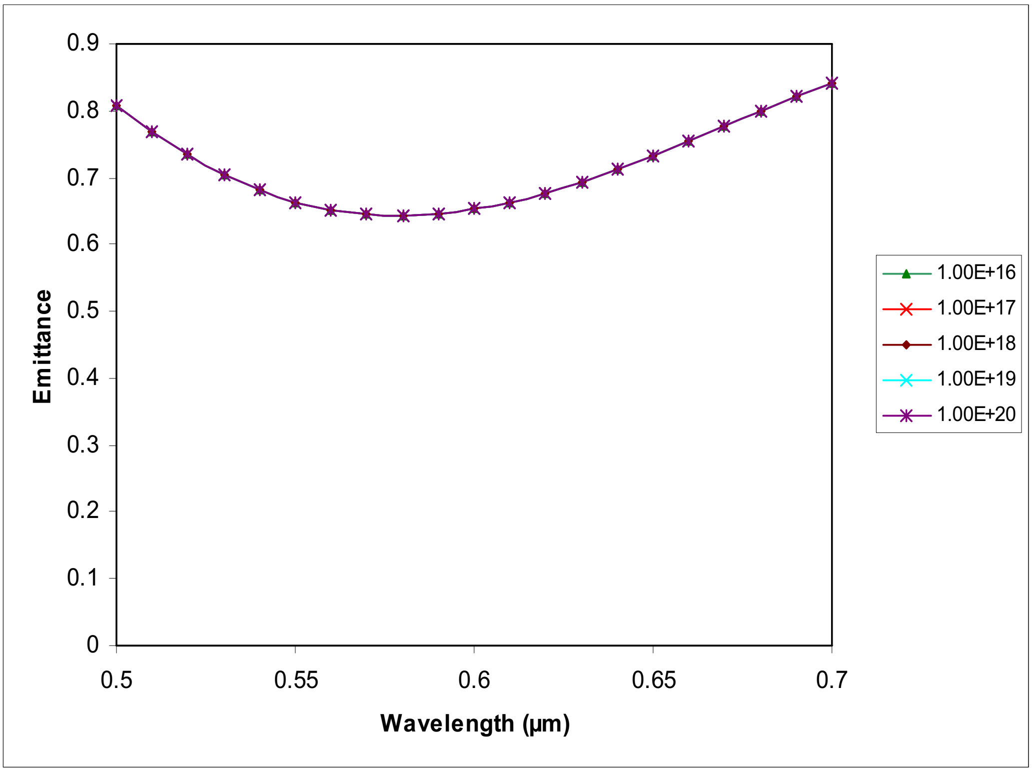

Fig. 9 Spectral Emittance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (p-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

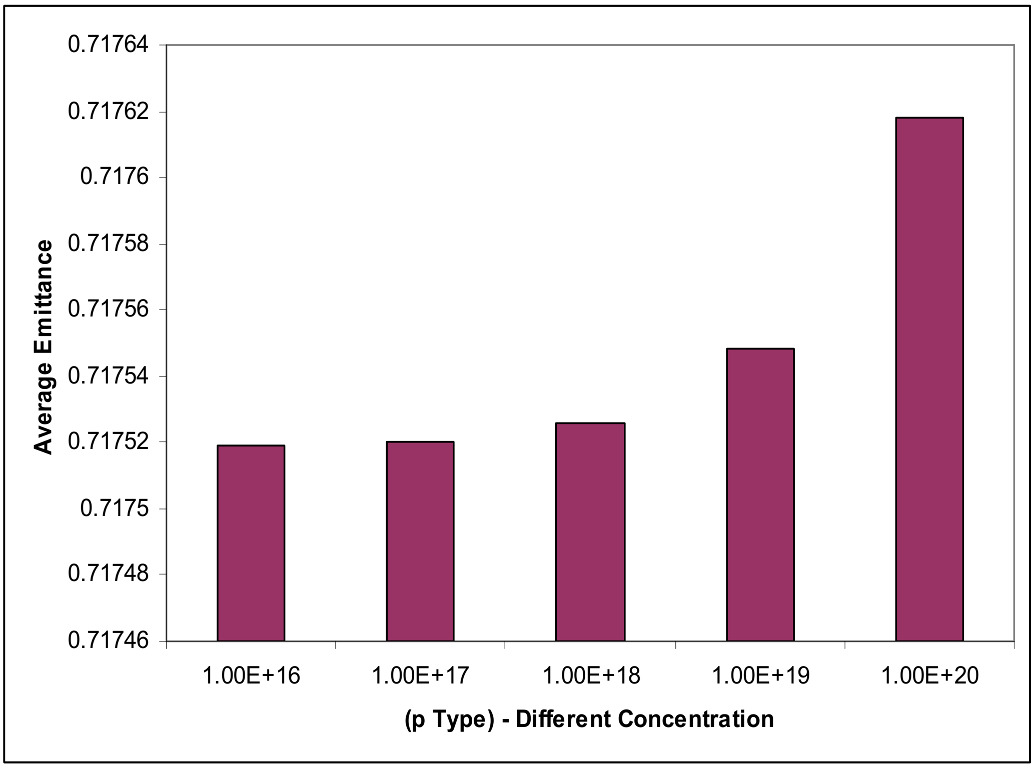

Fig. 10 Average Emittance of silicon wafer coated by silicon dioxide film on both sides with dopped silicon (p-type) in different concentrations, at room Temperatures and normal incidence for visible wavelengths

The oscillation in the radiative properties 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 thicker silicon dioxide film. Therefore oscillations increased toward longer wavelengths. Interferences in the substrate are generally not observable in the incoherent formulation. This is the major difference between coherent and incoherent formulations [6].

For visible wavelengths, more emittance occurs in greater concentrations and the reflectance decreases as the concentration increases. In these wavelengths, transmittance is negligible.

Donars and acceptors act similar in visible wavelengths.

At room temperature for concentration less than $10^{19}\, cm^{-3}$, concentration has not important influence on radiative properties.

At room temperature, the scattering process is dominated by lattice scattering for lightly doped silicon, and the impurity scattering becomes important for heavily doped silicon when the dopant concentration exceeds $10^{18}\, cm^{-3}$.

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