Effects of Donors and Acceptors on Radiative Properties of Nanoscale Multilayer Structures at Infrared Wavelengths

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Abstract: - Infrared imaging is used extensively for both military and civilian purposes using radiative properties of silicon and other relevant materials. Military applications include target acquisition, surveillance, night vision, homing and tracking. Non-military uses include thermal efficiency analysis, remote temperature sensing, short-ranged wireless communication, spectroscopy, and weather forecasting. This work uses the transfer-matrix method for calculating the radiative properties of silicon. For this purpose, doped silicon is used, the coherent formulation is applied, and the Drude model for the optical constants of doped silicon is employed. Results show that average reflectance changes from 0.3015 to 0.2060 for donor concentrations of $10^{17}cm^{-3}$ and $10^{19}cm^{-3}$, respectively, indicating that average reflectance decreases with increasing concentration. A donor concentration of $10^{19}cm^{-3}$ yields an average emittance of about 2.46 times higher than that yielded by a concentration level of $10^{17}cm^{-3}$. An acceptor concentration of $10^{19}cm^{-3}$ has an average emittance of about 2.14 higher than that of a concentration equal to $10^{17}cm^{-3}$. At infrared wavelengths, lower reflectance occurs at higher concentrations and emittance increases with increasing concentration. Results also show that donors and acceptors act similarly with respect to spectral radiative properties at infrared wavelengths.

Key-Words: Donors- Acceptors- Nanoscale- Multilayer- Infrared Wavelength

1 Introduction

The radiative properties of semiconductors are important in advancement of some manufacturing technologies such as rapid thermal processing [1]. Since the major heating source in the rapid thermal processing is lamp radiation, the knowledge of radiative properties is important in temperature control during the process. Silicon is a semiconductor that plays a vital role in integrated circuits and in MEMS/NEMS [2]. Semitransparent crystalline silicon solar cells can improve the efficiency of solar power generation [3]. Accurate radiometric temperature measurement 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]. Infrared imaging is used extensively for both military and civilian purposes. For lightly doped silicon that silicon dioxide coating has a higher reflectance than silicon nitride coating at visible wavelengths, where reflectance increases with increasing temperature due to decreasing emittance. At infrared wavelengths, however, the reflectance and transmittance decrease as temperature increases [2, 5]. The present study aims to determine the radiative properties of silicon using the transfer-matrix method. For this purpose, doped silicon is used and the coherent formulation and the drude model for the optical constants of doped silicon are employed. Phosphorus and boron are the default impurities of n- and p-types, respectively.

2 Modeling

2.1 Coherent Formulation

The transfer-matrix method provides a convenient way to calculate the radiative properties of the

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multilayer structure of thin films (Figure 1). 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

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

here, A_j and B_j are the amplitudes of forward and backward waves in the jth layer. Detailed descriptions of how to solve Eq. (1) for A_j and B_j is given in [6].

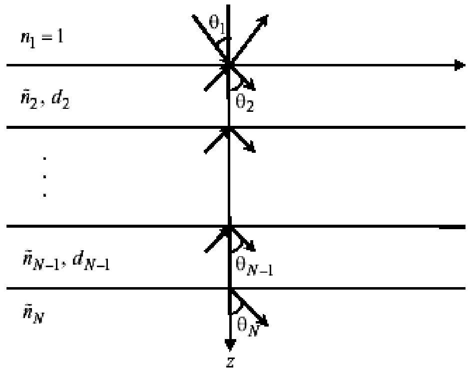

Figure 1: The geometry for calculating the radiative properties of a multilayer structure

Consequently, the radiative properties of the *N*-layer system are given by [1, 6]

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

2.2. Optical Constants

The Drude Model for the Optical Constants of Doped Silicon

To account for doping effects, the Drude model is employed, and the dielectric function of both intrinsic and doped silicon is expressed as follows [7]:

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

The scattering time, τ_e or τ_h, depends on the collisions of electrons or holes with the lattice (phonons) and the ionized dopant sites (impurities or defects); hence, it generally depends on 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 [8]:

$$\frac{1}{\tau_e} = \frac{1}{\tau_{e-l}} + \frac{1}{\tau_{e-d}} \quad (4)$$

where, τ_{e-l} and τ_{e-d} denote the electron-lattice and the electron-defect scattering times, respectively. Similarly, τ_h can be related to τ_{h-l} and τ_{h-d}. In addition, the scattering time, τ, is also related to mobility, μ, by the following relation:

$$\tau = m^* \mu / e \quad (5)$$

At room temperature, the total scattering time τ_e^0 or τ_h^0, which depends on the dopant concentration, can be determined from the fitted mobility equations [6]:

$$\mu_e^0 = \frac{1268}{1 + (N_D / 1.3 \times 10^{17})^{0.91}} + 92 \quad (6)$$

$$\mu_h^0 = \frac{447.3}{1 + (N_A / 1.9 \times 10^{17})^{0.76}} + 47.7 \quad (7)$$

where, the superscript 0 indicates values at 300 ºK and N_D is the dopant concentration of the donor (phosphorus, n-type) in cm^{-3}. Because of the relative insignificance of impurity scattering at high temperatures, the following formula will be used to calculate the impurity scattering times:

$$\frac{\tau_{e-d}}{\tau_{e-d}^0} = \frac{\tau_{h-d}}{\tau_{h-d}^0} = \left(\frac{T}{300}\right)^{1.5} \quad (8)$$

Detailed descriptions of semiconductor devises are given in Ref.9. The optical constants of silicon dioxide are mainly based on the data collected in Palik [10].

3 Results

Figure 2 compares the emittance of doped silicon with donors and concentration of $1\times10^{18} cm^{-3}$ with the dioxide silicon thin film coating in the different temperatures with the results in [11]. The silicon thickness is $700\mu m$ and the thickness of the dioxide silicon is $65.3nm$ and the Electromagnetic waves are incident at $\theta = 0^\circ$. The calculated results are in good agreement with results in [11].

Now consider the case in which the silicon wafer is coated with a silicon dioxide layer on both sides. The thickness of the silicon wafer is $500\mu m$, the temperature of the silicon wafer with thin-film coatings is 25ºC, and the electromagnetic waves are incident at $\theta = 0^\circ$. The wavelength range considered is $0.7\mu m < \lambda < 2\mu m$. Doped 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. Phosphorus acts as the donor (n-type) and boron acts as the acceptor (p-type) for doped silicon.

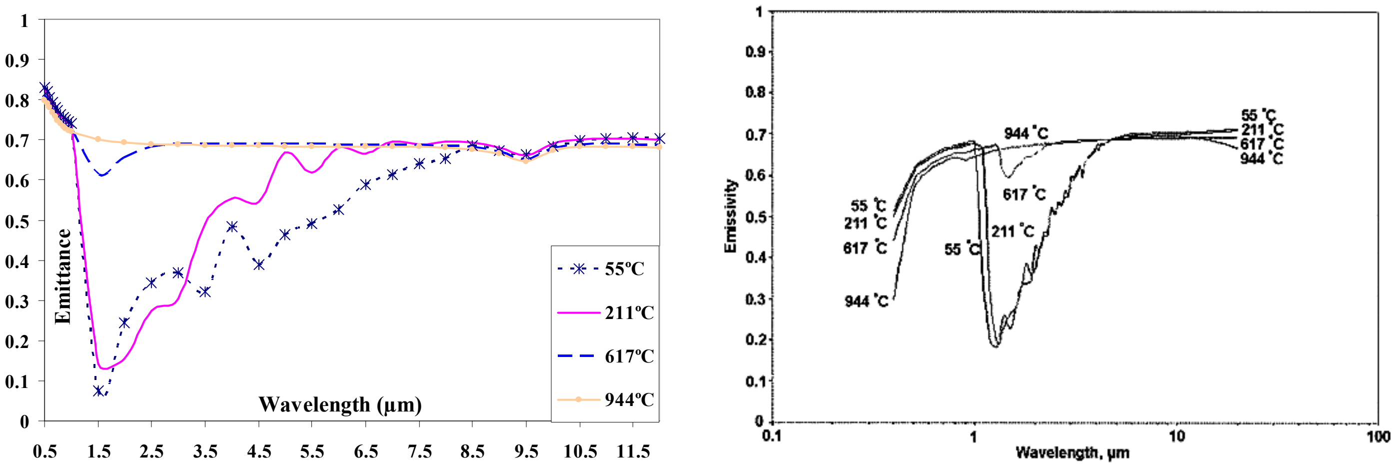

Figure 2. A comparison of the calculated results (Left side) with results of [11] (Right side)

Impurity concentration varies from $10^{17}cm^{-3}$ to $10^{19}cm^{-3}$. The Electromagnetic waves are incident at $\theta = 0^{\circ}$ and layers at room temperature. Some of the results obtained are shown in Figures 3 to 8 and tables 1 to 3 below.

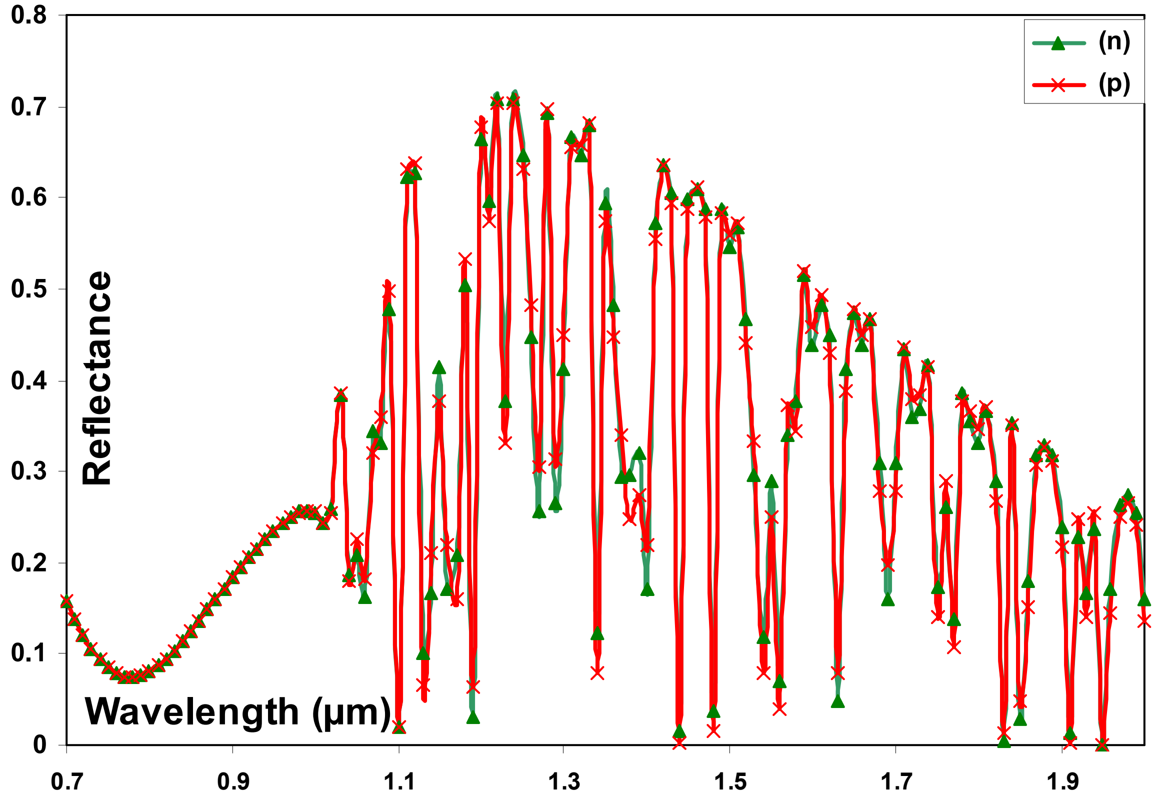

Figure 3. Spectral reflectance of silicon wafer coated with a silicon dioxide film on both sides with a doped silicon concentration of $10^{17}cm^{-3}$

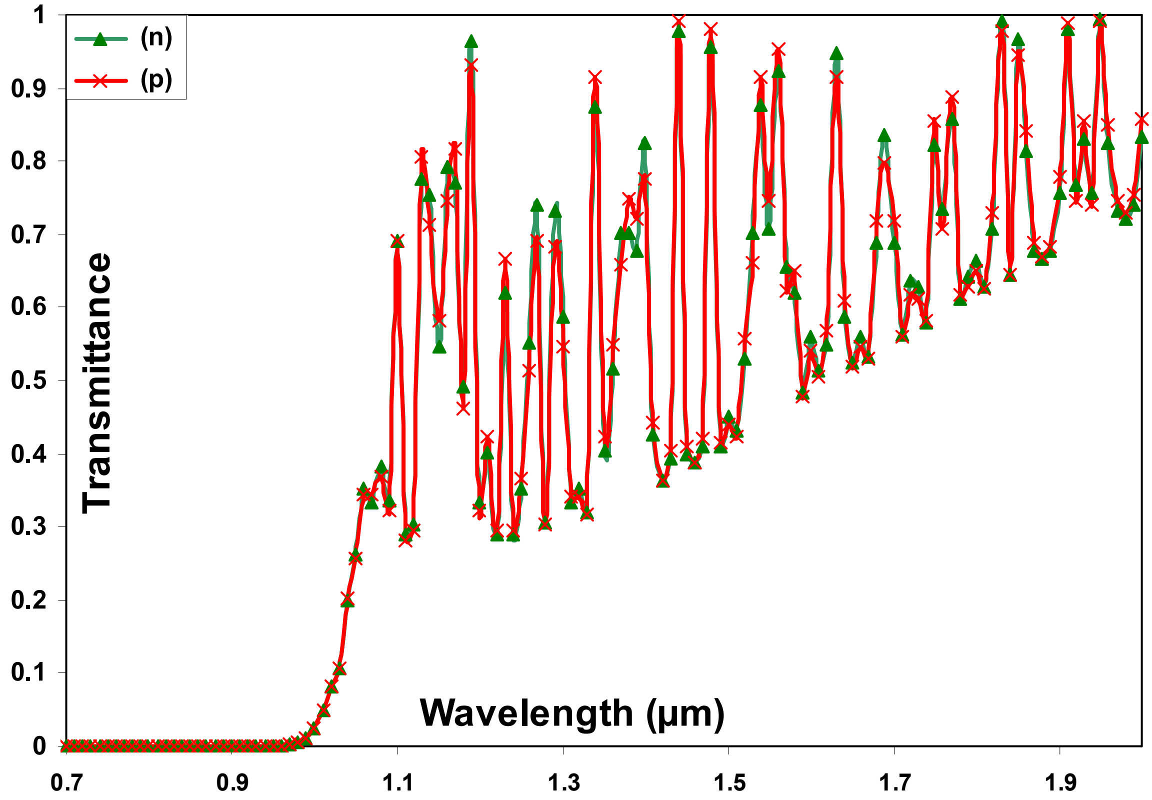

Figure 4. Spectral transmittance of a silicon wafer coated with a silicon dioxide film on both sides with a doped silicon concentration of $10^{17}\,cm^{-3}$

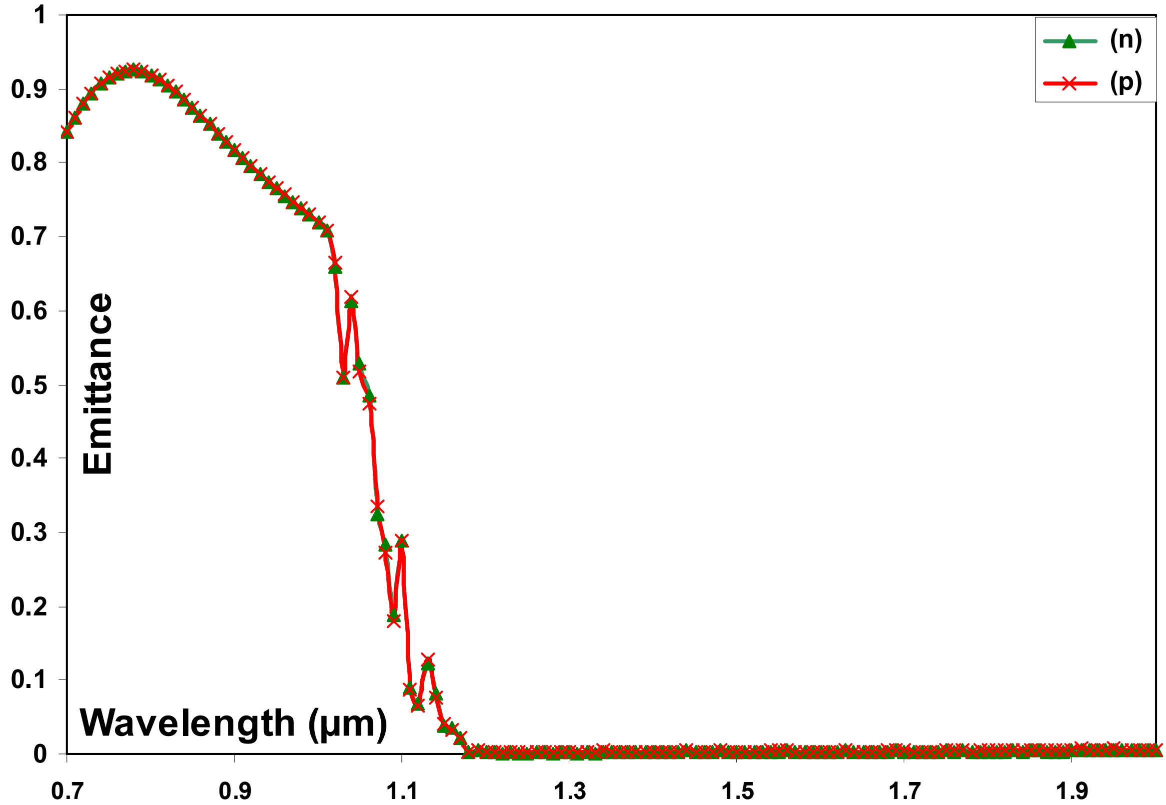

Figure 5. Spectral emittance of a silicon wafer coated with a silicon dioxide film on both sides with a doped silicon concentration of $10^{17}\,cm^{-3}$

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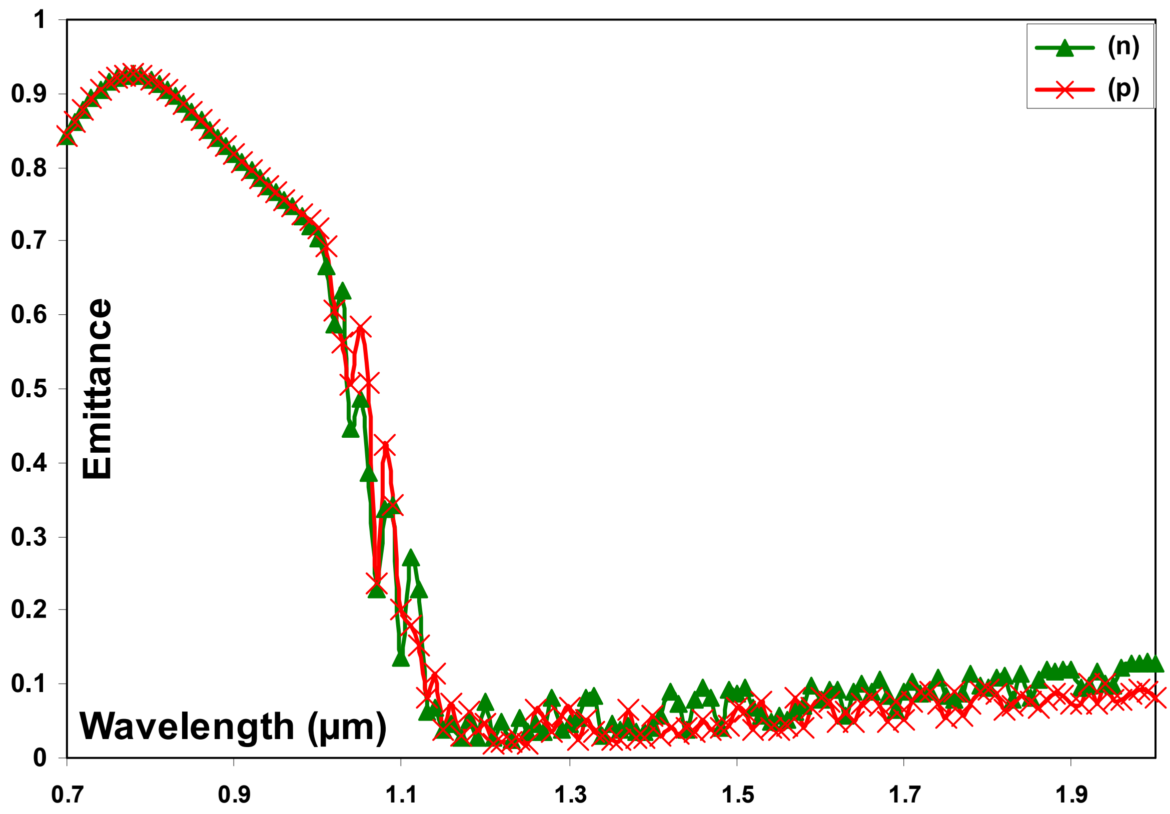

Figure 6. Spectral emittance of a silicon wafer coated with a silicon dioxide film on both sides with a doped silicon concentration of $10^{18}cm^{-3}$

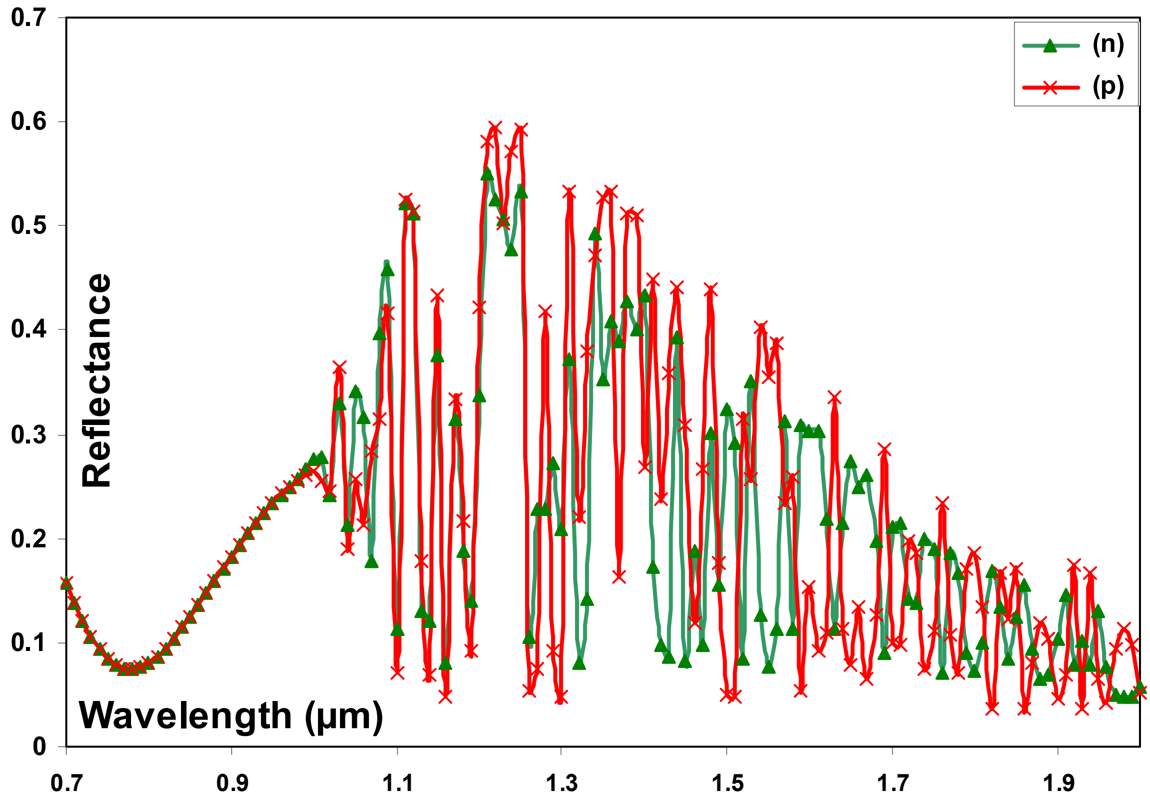

Figure 7. Spectral reflectance of a silicon wafer coated with a silicon dioxide film on both sides with a doped silicon concentration of $10^{19}cm^{-3}$

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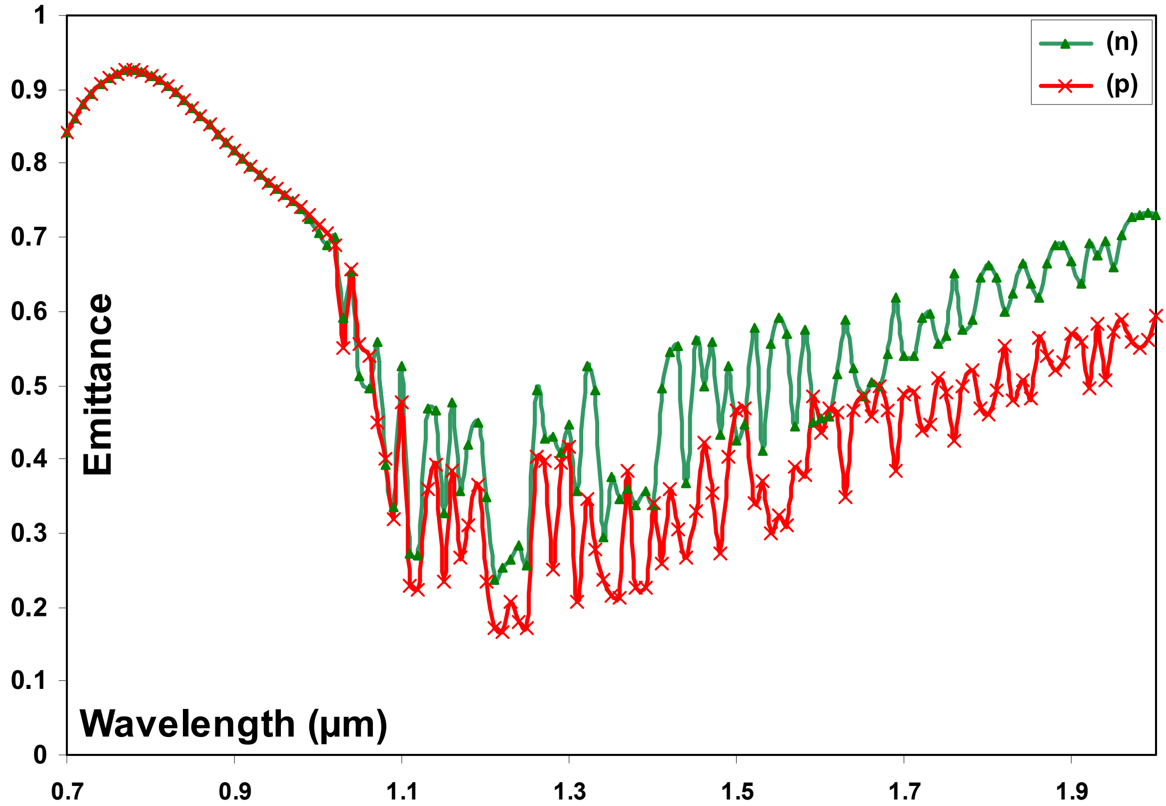

Figure 8. Spectral emittance of a silicon wafer coated with a silicon dioxide film on both sides with a doped silicon concentration of $10^{19} cm^{-3}$

Table1. Average Reflectance of a doped silicon wafer coated with a silicon dioxide film on both sides

Impurity Type / concentration	$10^{17} cm^{-3}$	$10^{18} cm^{-3}$	$10^{19} cm^{-3}$
Donar Impurity	0.3015	0.2496	0.2060
Acceptor Impurity	0.3000	0.2687	0.2135

Table2. Average Transmittance of a doped silicon wafer coated with a silicon dioxide film on both sides

Impurity Type / concentration	$10^{17} cm^{-3}$	$10^{18} cm^{-3}$	$10^{19} cm^{-3}$
Donar Impurity	0.4580	0.4626	0.2019
Acceptor Impurity	0.4590	0.4528	0.2727

Table3. Average Emittance of a doped silicon wafer coated with a silicon dioxide film on both sides

Impurity Type / concentration	$10^{17} cm^{-3}$	$10^{18} cm^{-3}$	$10^{19} cm^{-3}$
Donar Impurity	0.2406	0.2878	0.5921
Acceptor Impurity	0.2409	0.2785	0.5138

4 Conclusion

The effect of wave interference can be understood by plotting such spectral properties 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 [2, 5]. Interferences in the substrate are generally not observable in the incoherent formulation. This is the major difference between coherent and incoherent formulations [5].

Results showed that the average reflectance for a dopant concentration of $10^{17}cm^{-3}$ is 0.3015 for donors, and 0.30 for acceptors. The average reflectance for a dopant concentration of $10^{19}cm^{-3}$ is 0.2060 for donors, and 0.2135 for acceptors. Average reflectance changed from 0.3015 to 0.2060 for donor concentrations of $10^{17}cm^{-3}$ and $10^{19}cm^{-3}$, respectively. It may be concluded that average reflectance decreases with increasing concentration.

It was also observed that the average emittance for a dopant concentration of $10^{17}cm^{-3}$ is 0.2406 for donors, and 0.2409 for acceptors. This is while the average emittance values for a dopant concentration of $10^{19}cm^{-3}$ are 0.5921 and 0.5138 for donors and acceptors, respectively.

A donor concentration of $10^{19}cm^{-3}$ yields an average emittance around 2.46 times greater than that yielded by a concentration of $10^{17}cm^{-3}$. An acceptor concentration of $10^{19}cm^{-3}$ yields an average emittance about 2.14 times greater than that by a concentration of $10^{17}cm^{-3}$.

In the case of infrared wavelengths, less reflectance occurs at greater concentrations with emittance increasing as concentration increases. The results obtained from the present study revealed that donors and acceptors act similarly for spectral radiative properties at the infrared wavelengths.

At room temperature and at concentration levels below $10^{19}cm^{-3}$, concentration has no significant effect on radiative properties. Scattering process at room temperature is dominated by lattice scattering for lightly doped silicon, while impurity scattering at the same temperature becomes important for heavily doped silicon when the dopant concentration exceeds $10^{18}cm^{-3}$. Therefore, coatings act as wavelength selective emitters for radiative energy conversion and thermal radiation detection.

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