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Parametric Study of Nanoscale Radiative Properties of Doped Silicon Multilayer Structures

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Abstract: Thin film coatings play an important role in the semiconductor industries and micro electromechanical and nano electromechanical equipments. In this paper, the doped silicon with donors and acceptors with different concentrations are studied and the dioxide silicone thin film is compared at different temperatures. From the results, 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 $1\times10^{16}\text{cm}^{-3}$. By increasing temperature, a lattice scattering phenomenon becomes dominant because of increasing the concentration of the phonons. For higher temperatures, this effect is reduced due to faster movement of energy carriers and a decrease in the Coulomb force between ions. More interestingly, it is observed from the results that the reflectance for the wavelength about 400*nm* in the most cases is constant which offers a good choice for filtering ultraviolet waves.

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Key words: Doped Silicon % Donors % Acceptors % Nanoscale % Concentration and Temperature

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]. In fact, surface modification by coatings can significantly affect the radiative properties of a material [5, 6]. 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 [5]. This work uses transfer-matrix method for calculating the radiative properties. Doped 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.

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

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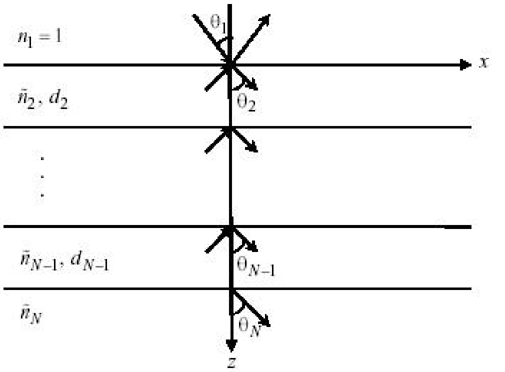

Fig. 1: The geometry for calculating the radiative properties of a multilayer structure

properties of the multilayer structure of thin films (Figure 1). Assuming that the electromagnetic 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

$$E_j\begin{cases}\left[A_1e^{iq1z^z}+B_1e^{-iq1z^z}\right]e^{(iq_xx-iwt)},\ j=1\\ \left[A_je^{iq_{jz}(z-z_{j-1})}+B_je^{-iq(z-z_{j-i})}\right]e^{(iq_xx-iwt)},\ j=2,3,...N\end{cases}\quad(1)$$

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

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 [7]. Li [8] 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 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 [7]. 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 [1]:

$$"(8,T)="_{BG}(8,T)+"_{FC}(8,T)\quad(2)$$

The expression for the band gap absorption can be found in the work by MarcFalane *et al*. [9, 10]. For free-carrier absorption, Sturm and Reaves [11] suggested an expression. Vandenabeele and Maex [12] 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

$$a_{FC}(l,T)=4.15\times10^{-5}\,l^{1.51}(t+273.15)^{2.95}\exp\left(\frac{-7000}{T+273.15}\right)\quad(3)$$

Rogne *et al.* [13] 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. The optical constants of silicon dioxide are mainly based on the data collected in Palik [14].

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 (6) by $g(T)=(n+ik)^2$. To account for doping effects, the Drude model is employed and the dielectric function of both intrinsic and doped silicon is expressed as follows [15]:

$$e(w)=e_{bl}-\frac{N_ee^2/e_0m_e^*}{w^2+iw/t_e}-\frac{N_he^2/e_0m_h^*}{w^2+iw/t_h}\quad(4)$$

The values for the effective density of states at room temperature are found in [16]. The Fermi-Dirac integral $F_{1/2}$ can be simplified by an exponential and the procedures described in [17] are used to determine the Fermi energy satisfying charge neutrality. The ionization energies of phosphorus and boron values are taken from [18]. The scattering time, J_e or J_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 J_e), which consists of the above two mechanisms, can be expressed as [19]:

$$\frac{1}{t_e}=\frac{1}{t_{e-l}}+\frac{1}{t_{e-d}}\quad(5)$$

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

$$J = m^{*}\mu/e \tag{6}$$

At room temperature, the total scattering time t_e^0 or t_h^0, which depends on the dopant concentration, can be determined from the fitted mobility equations [19]:

$$m_e^0 = \frac{1268}{1+(N_D/1.3\times10^{17})^{0.91}}+92 \tag{7}$$

$$m_h^0 = \frac{447.3}{1+(N_A/1.9\times10^{17})^{0.76}}+47.7 \tag{8}$$

where, the superscript 0 indicates values at 300 °K and N_D or N_A is the dopant concentration of the donor (phosphorus, n-type) or the acceptor (boron, p-type) in cmG^3. On the other hand, the scattering time from the lattice contribution t_{e-l}^0 or t_{h-l}^0, are given in [11]. Because of the relative insignificance of impurity scattering at high temperatures, the following formula will be used to calculate the impurity scattering times:

$$\frac{t_{e-d}}{t_{e-d}^0} = \frac{t_{h-d}}{t_{h-d}^0} = \left(\frac{T}{300}\right)^{1.5} \tag{9}$$

In order to obtain a better agreement with the measured near-infrared absorption coefficients for lightly doped silicon [1, 11-13], the expressions for lattice scattering are modified in the present study as follows:

$$t_{e-l} = t_{e-l}^0 (T/300)^{-3.8} \tag{10}$$

$$t_{h-l} = t_{h-l}^0 (T/300)^{-3.6} \tag{11}$$

RESULTS AND DISCUSSION

Figure 2 compares the emittance of doped silicon with donors and concentration of 1×10^{18} *cm*G^3 with the dioxide silicon thin film coating in the different temperatures with the results in [20]. The silicon thickness is 700*µm* and the thickness of the dioxide silicon is 65.3*nm* and the Electromagnetic waves are incident at 2 = 0. The calculated results are in good agreement with results in [20]. Figure 3 shows the reflectance and transmittance of doped silicon with donors and 1×10^{18} *cm*G^3 concentration with silicon dioxide coating at different temperatures. Figure 4 shows the emittance and reflectance of doped silicon with donors and different concentrations coated by silicon dioxide at the same condition of figure 2 but in the 944°C temperature. Figure 5 shows the emitance and reflectance of doped silicon with donors and acceptors in the different concentrations with silicon dioxide coating and the same conditions of figure 2 but in the 211°C temperature.

From the Results:

C 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.

C The reflectance and the transmittance decrease as the temperature increases, because of increasing absorbance (Figure 3).

C As the Figure 3 shows, silicon in the high temperatures act like an opaque medium and so the reflectance in high temperatures reaches to zero.

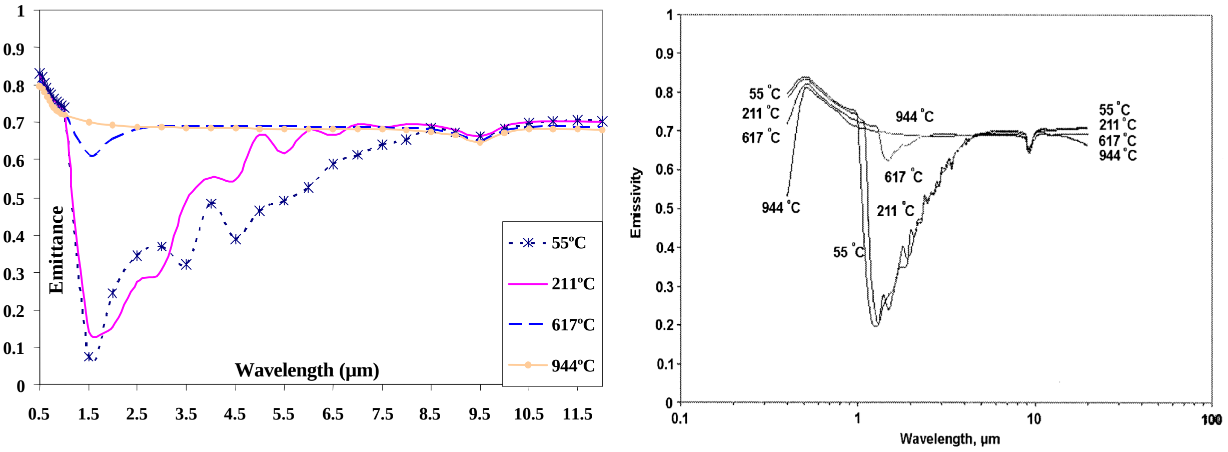

Fig. 2: A comparison of the calculated results (Left side) with results of [20] (Right side)

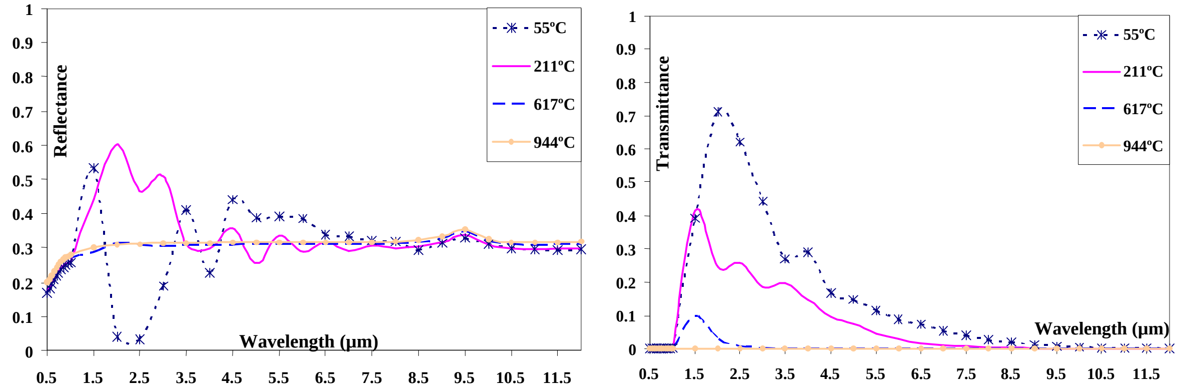

Fig. 3: Reflectance and Transmittance of doped silicon multilayer at different temperatures

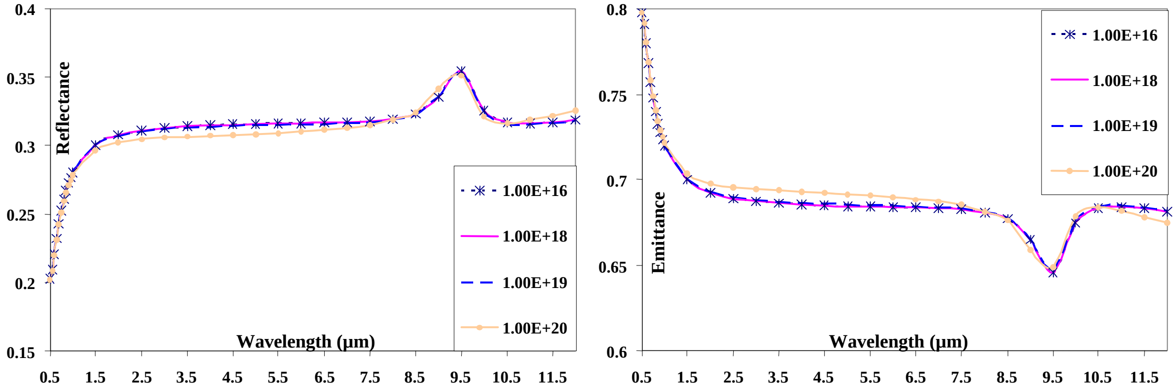

Fig. 4: Reflectance and Emittance of doped silicon multilayer with donors and different concentrations (cmG^3) at 944°C

- The results showed that the transmittance in the temperatures greater than 617°C is independent of the wavelength. Also changing in the coating and concentrations, have not any effect on the total emittance, because the opaque behavior appears in these temperatures.
- The results showed that the reflectance for the wavelength around 400*nm* become constant and it is possible to use this structure as a good filter for the ultraviolet area (Figure 3).
- The differences between the emittance cleared in the smaller wavelengths, but it is not observable in infrared wavelengths when increasing the wavelength to 9 µm (Figure 2).
- The results showed that increasing concentration at 994°C temperature, leads to the partial reduction in the reflectance and partial increasing in the emittance (Figure 4).
- It was also observed from the figure 4 that the effect of the concentration on the radiative properties in the high temperatures is low.
- The emittance in the infrared spectrum for wavelength more than 10μm, reaches to 0.67(Figure4).
- When ever the temperature increases, the lattice scattering would be dominant because of the increasing of phonon's concentration and in the higher temperatures, the importance of scattering by ions is reduced; because in the high temperatures, the energy carriers move faster and the coulomb force decreases between them. For temperature greater than 600°*K*, the scattering time is being the same for the different concentrations (Figure 4).
- The results of the figure 5 were showed that increasing of the concentration leads to the increasing of emittance and reduction of attraction coefficient in the 211°C temperature. These behaviors are similar for both donor and acceptor impurities.
- In high concentrations, donors have greater emittanc and the smaller reflectance than the acceptors. So the concentration effect on the radiative properties for temperatures lower than 600°*K* is high (Figure 5).
- Effect of doped ions for low concentrations is not considerable, so the ions effects in the scattering time become apparent for the concentrations more than 1×10^{16}*cm*G^3 (Figure 5).

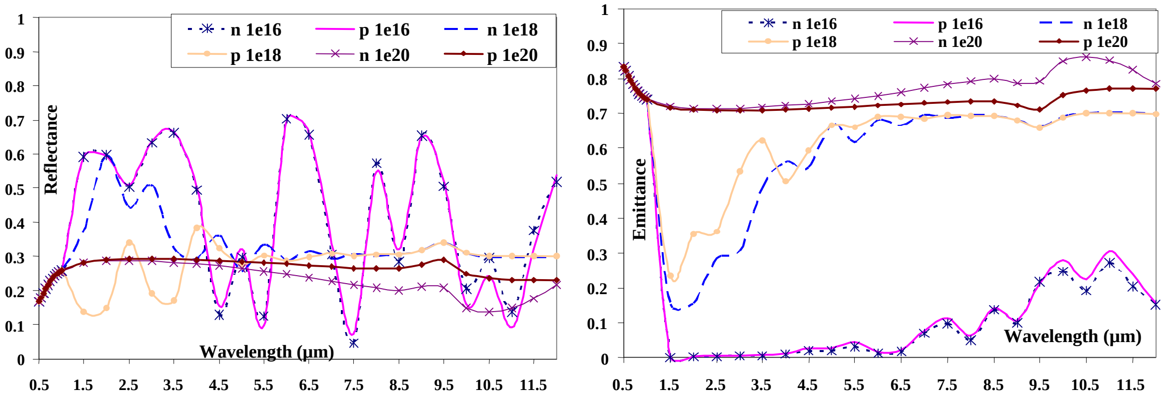

Fig. 5: Reflectance and Emittance of doped silicon multilayer with donors and acceptors at different concentrations (cm^{-3}) in 211°C

- Results indicated that for concentration less than $1\times10^{18}cm^{-3}$, donors have lower average emittance and greater average reflectance than acceptors (Figure 5).

REFERENCES

1. Timans, P.J., 1996. The Thermal Radiative Properties of Semiconductors Advances in Rapid Thermal and Integrated Processing, Academic Publishers, Dordrecht, Netherlands, pp: 35-102.
2. Makino, T., 2002. Thermal Radiation Spectroscopy for Heat Transfer Science and for Engineering Surface Diagnosis, In: Taine J editor. Heat transfer, 1. Oxford: Elsevier Science, pp: 55-66.
3. Fath, P., H. Nussbaumer and R. Burkhardt, 2002, Industrial Manufacturing of Semitransparent Crystalline Silicon Power Solar Cells. Sol Energy Mater Sol Cells, 74: 127-131.
4. Makino, T., 2002. Thermal radiation spectroscopy for heat transfer science and for engineering surface diagnosis, In: Taine J. editor. Heat transfer, 1. Oxford: Elsevier Science, pp: 55-66.
5. Oloomi, S.A.A., A. Sabounchi and A. Sedaghat, 2009. Computing Thermal Radiative Properties of Nanoscale Multilayer, World Academy of Science, Engineering and Technology, 37: 929-934.
6. Zhang, Z.M., C.J. Fu and Q.Z. Zhu, 2003. Optical and Thermal Radiative Properties of Semiconductors Related to Micro/Nanotechnology, Advanced in Heat Transfer, 37: 179-296.
7. Jellison, G.E. and F.A. Modine, 1994. Optical Functions of Silicon at Elevated Temperatures, J. Appl. Phys., 76: 3758-3761.
8. Li, H.H., 1980. Refractive Index of Silicon and Germanium and Its Wavelength and Temperature Derivatives, J. Phys. Chem. Ref. Data, 9: 561-658.
9. Macfarlane, G.G., T.P. Mclean, J.E. Quarrington and V. Roberts, 1958. Fine Structure in the Absorption-Edge Spectrum of Si, Phys. Rev., 111: 1245-1254.
10. Timans, P.J., 1993. Emissivity of Silicon at Elevated Temperatures, J. Appl. Phys., 74: 6353-6364.
11. Sturm, J.C. and C.M. Reaves, 1992. Silicon Temperature-Measurement by Infrared Absorption Fundamental Processes and Doping Effects, IEEE Trans. Electron Devices, 39: 81-88.
12. Vandenabeele, P. and K. Maex, 1992. Influence of Temperature and Backside Roughness on the Emissivity of Si Wafers during Rapid Thermal-Processing, J. Appl. Phys., 72: 5867-5875.
13. Rogne, H., P.J. Timans and H. Ahmed, 1996. Infrared Absorption in Silicon at Elevated Temperatures, Appl. Phys. Lett., 69: 2190-2192.
14. Palik, E.D., 1998. Silicon Dioxide (SiO2), Handbook of Optical Constants of Solids, San Diego, CA., pp: 749-763.
15. Hebb, J.P., 1997. Pattern Effects in Rapid Thermal Processing, Cambridge, MA.
16. Sze, S.M., 2002. Semiconductor Devices, Physics and Technology, 2nd Ed, Wiley, New York.
17. Sze, S.M., 1981, Physics of Semiconductor Devices, 2nd Ed, Wiley, New York.
18. Beadle, W.E., J.C.C. Tsai and R.D. Plummer, 1985. Quick Reference Manual for Silicon Integrated Circuit Technology, Wiley, New York.
19. Morin, F.J. and J.P. Maita, 1954. Electrical Properties of Silicon Containing Arsenic and Boron, Phys. Rev., 96: 28-35.
20. Ravindra, N.M. et al., 2001. Emissivity Measurements and Modeling of Silicon-Related Materials, Intl. J. Thermophysics, 22(5): 1593-1611.