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Effects of incidence polarization on radiative properties of doped silicon multilayer structures

S. A. A. Oloomi^{*}, A. Saboonchi and A. Sedaghat

Department of Mechanical Engineering, Isfahan University of Technology, Isfahan, 84156-83111, I. R. of Iran.

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Study of the surfaces which covered by thin films are very important. In this paper, the doped silicon with donors and acceptors with different concentrations coated by silicon dioxide and different polarization incident angles are studied. Results show that effect of doped ions for low concentrations is not considerable, so the ion effects in the scattering time become apparent for the concentrations more than. Results also show that the difference between S-polarization and P-polarization increases with increasing of incidence angle. The reflectance of S-polarization is greater than the reflectance of P-polarization. When the incident radiation is unpolarized, the radiative properties are averaged over p and s polarizations. Thermal radiaitive properties of nanoscale multilayer structures strongly depend on impurity types and incidence polarization. Therefore industrial requirements are supported by selecting donors or acceptors and s or p incidence polarization.

Key words: Doped silicon, incidence angle, nanoscale, P-polarization, radiative properties, S-polarization.

INTRODUCTION

The radiative properties of semiconductors are important in advancement of some manufacturing technologies such as rapid thermal processing (Timans, 1996). 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 (Oloomi et al., 2009a). Effect of doped ions on radiative properties of nanoscale multilayer structures must be considered. This work uses coherent formulation for calculating the radiative properties of semiconductor materials related to the recent technological advancements that are playing a vital role in the integrated-circuit manufacturing, optoelectronics, and radiative energy conversion devices. 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 ptype, respectively in this work. This paper considered the effects of donors and acceptors on radiative properties of

nanoscale multilayer structures.

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 (Timans., 1996; Zhang et al., 2003):

$$E_{j} = \begin{cases} \left[A_{1}e^{iq_{1z}z} + B_{1}e^{-iq_{1z}z}\right]e^{(iq_{x}x - i\omega t)}, \ j = 1\\ \left[A_{j}e^{iq_{jz}(z - z_{j-1})} + B_{j}e^{-iq_{jz}(z - z_{j-1})}\right]e^{(iq_{x}x - i\omega t)}, \ j = 2,3,...N \end{cases}$$
(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 equation (1) for A_j and B_j is given in Timans (1996) and Zhang et al. (2003). Consequently, the radiative properties of the *N*-layer system such as reflectance ρ , transmittance τ and emittance ε are

^{*}Corresponding author E-mail : AmirOloomi@me.iut.ac.ir.



Figure 1. A comparison of the calculated results (Left side) with results of (Ravindra et al., 2001) (Right side).

given by (Timans., 1996; Zhang et al., 2003):

The coefficients of adjacent layers are related by

$$\binom{A_j}{B_j} = P_j D_j^{-1} P_j \binom{A_{j+1}}{B_{j+1}}, (j = 1, 2, 3, ..., N - 1)$$
(2)

where asterisks denote the complex conjugate.

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 (Timans., 1996; Zhang et al., 2003):

where P_i is the propagating matrix:

$$P_{1} = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, P_{j} = \begin{pmatrix} e^{-iq_{k}d_{j}} & 0 \\ 0 & e^{+iq_{k}d_{j}} \end{pmatrix}, (j = 2, 3, ..., N - 1)$$
(3)

The scattering time, \mathcal{T}_e or \mathcal{T}_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 \mathcal{T}_e), which consists of the above two mechanisms, can be expressed as (Beadle et al., 1985):

 D_i is the transfer matrix given below and D_i^{-1} is its inverse.

$$D_{j} = \begin{pmatrix} 1 & 1 \\ n_{j} \cos \theta_{j} & -n_{j} \cos \theta_{j} \end{pmatrix}, (j = 1, 2, 3, \dots, N-1)_{\text{for a}}$$
TE wave (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

 T_{h-l} and T_{h-d} . In addition, the scattering time, τ , is also related to mobility, μ , by the following relation:

$$D_{j} = \begin{pmatrix} \cos \theta_{j} & \cos \theta_{j} \\ n_{j} & -n_{j} \end{pmatrix}, (j = 1, 2, 3, ..., N - 1) \text{ for a TM wave}$$
(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 (Timans., 1996; Zhang et al., 2003):

Hence,

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M \begin{pmatrix} A_N \\ B_N \end{pmatrix}, \ M = \prod_{j=1}^{N-1} P_j D_j^{-1} D_{j+1}$$
(6)

$$\rho = \frac{B_1 B_1^*}{A_1^2}, \tau = \frac{\operatorname{Re}(\tilde{n}_N \cos \tilde{\theta}_N)}{n_1 \cos \theta_1} \frac{A_N A_N^*}{A_1^2}, \varepsilon = 1 - \rho - \tau$$
(7)

where superscript 0 indicates values at 300 % and N_D or N_A is the dopant concentration of donor (Phosphorus, n-type) or acceptor (Boron, p-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:

$$\varepsilon(\omega) = \varepsilon_{bl} - \frac{N_e e^2 / \varepsilon_0 m_e^*}{\omega^2 + i\omega / \tau_e} - \frac{N_h e^2 / \varepsilon_0 m_h^*}{\omega^2 + i\omega / \tau_h}$$
(8)

Detailed descriptions of semiconductor devises are given in Sze (2002). The optical constants of silicon dioxide are mainly based on the data collected in Palik (1998).

RESULTS AND DISCUSSION

Figure 1 compares the emittance of donor doped silicon with concentration of $1 \times 10^{18} cm^{-3}$ coated by silicon



Figure 2. Reflectance and emittance of doped silicon multilayer with donors and acceptors at different concentrations (cm³) in 211 °C.



Figure 3. Reflectance of donors doped silicon multilayer with S and P polarizations in different incidence angle and room temperature.

dioxide in the different temperatures with the results in Ravindra et al. (2001). The silicon thickness is 700 μm and the thickness of the dioxide silicon is 63.3 nm and the electromagnetic wave is incident at $\theta = 0^{\circ}$. The calculated results are in agreement with that of Ravindra et al. (2001). Figure 2 shows the reflectance and emittance of the doped silicon with donors and acceptors in different concentrations and coated by silicon dioxide with the same conditions as Figure 1. Figure 2 shows the properties at a temperature of 211 °C. 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 (Oloomi et al., 2010). Interferences in

the substrate are generally not observable in the incoherent formulation. This is the major difference between coherent and incoherent formulations (Oloomi et al., 2009b). Now consider the case that donor doped silicon with concentration of $1 \times 10^{18} cm^{-3}$ coated by silicon dioxide on both sides. The silicon thickness is 700 μ m and the thickness of the dioxide silicon is 65.3nm. Incidence ray is polarized. Figure 3 compares reflectance of nanoscale multilayer structures with S-polarization and P-polarization for different incidence angles at room temperature.

Any electromagnetic wave consists of an electric field component and a magnetic field component. The electric field component is used to define the plane of polarization



Figure 4. Transmittance of donors doped silicon multilayer with S and P polarizations in different incidence angle and room temperature

because many common electromagnetic-wave detectors respond to the electric forces on electrons in materials, not the magnetic forces.

Polarization is a characteristic of all transverse waves. Oscillations which take place in a transverse wave in many different directions are said to be unpolarized. In an unpolarized transverse wave, oscillations may take place in any direction at right angles to the direction in which the wave travels. Polarization of incident ray has strong effect on radiative properties of nanoscale multi-layer structure.

When the electric filed vector is perpendicular to the plane of incidence, the light is said to be S-polarized (TE). When the electric filed vector is parallel to the plane of incidence, the light is said to be P-polarized (TM). Figure 4 shows transmittance of nanoscale multilayer structures with S-polarization and P-polarization for different incidence angles at room temperature.

Figure 5 compares S-polarization and P-polarization for different incidence angles of nanoscale multilayer structures emittance in room temperature. From the results:

1. 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.

2. The differences between the emittance are clear in the smaller wavelength range, but it is not observable in infrared range when increasing the wavelength to 9 μm (Figure 1).

3. The results of the Figure 2 show that increasing of the concentration leads to the increasing of emittance and

reduction of attraction coefficient (not shown in Figure 2) in the 211 °C temperature. These behaviors are similar for both donor and acceptor impurities.

4. In high concentrations, donors have greater emittance and the smaller reflectance than the acceptors. So the concentration effect on the radiative properties for temperatures lower than $600 \,^{\circ}K$ is high (Figure 2).

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} $^{-3}$ (Figure 6)

$$1 \times 10^{10} cm^{-3}$$
 (Figure 2).

6. Results indicated that for concentration less than $1 \times 10^{18} cm^{-3}$, donors have lower average emittance and greater average reflectance than acceptors (Figure 2).

7. Results showed that in incidence angle of zero, radiative properties of S-polarization and P-polarization are equal. They are equal because of $\cos 0 = 1$. The transfer matrix for both S-polarization and P-polarization is equal. (From the Equations 4 and 5)

8. The difference between S-polarization and P-polarization increases with increasing of incidence angle (Figures 3 to 5).

9. Figure 3 shows that the reflectance of S-polarization is greater than the reflectance of P-polarization. Maximum of reflectance occurs for S-polarization in 60° of incidence angle, and P-polarization has minimum of reflectance.

10. The maximum of transmittance occurs for Ppolarization in 60° of incidence angle and S-polarization has minimum of transmittance (Figure 4). In generally transmittance of P-polarization is greater than it's Spolarization.



Figure 5. Emittance of donors doped silicon multilayer with S and P polarizations in different incidence angle and room temperature.

11. The results of the Figure 5 show that changing of incidence polarization from s to p, leads to the increasing of emittance. For example, in wavelength of 1.5 μm the emittance of P-polarization in 60° of incidence angle, is about 4.41 greater than S-polarization (Figure 5).

12. In wavelength of 9.5 μ m, minimum of reflectance is 0.10043 and occurs in P-polarization of incidence 60°. It changes to 0.57659 for S-polarization (Figure 3).

13. When the incident radiation is unpolarized, the radiative properties are averaged over p and s polarizations.

14. Thermal radiaitive properties of nanoscale multilayer structures strongly depend on impurity types and incidence polarization. Therefore industrial requirements are supported by selecting donors or acceptors and s or p incidence polarization.

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