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Estimation of optical parameters of silicon single crystals with different orientations

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Optical properties of Si single crystals with different orientations (1 0 0) and (1 1 1) were investigated using spectrophotometric measurements in a spectral range of 200 nm to 2500 nm. The data of optical absorption revealed an indirect allowed transition with energy gap of 1.1 ± 0.025 eV. An anomalous dispersion in addition to a normal dispersion was observed in the spectra of refractive index. The normal dispersion of the refractive index was discussed according to Wemple-DiDomenico single oscillator model. The oscillator energy E_o, dispersion energy E_d, high frequency dielectric constant ϵ_∞, lattice dielectric constant ϵ_L and electronic polarizability α_e were estimated. The real ϵ_1 and imaginary ϵ_2 parts of dielectric constant were also determined.

Keywords: *single crystals; different orientations; optical parameters*

1. Introduction

Silicon is a commonly used semiconductor in optoelectronic devices and photodiodes, which are broadly used in industrial applications as effective devices for light to electricity conversion [1]. The availability of high-quality single crystal and well-developed processing technologies stimulate new directions in investigations of the properties of silicon [2]. The field of research associated with optical properties of semiconductors has seen an enormous growth over the last decade [3]. The knowledge of optical material properties is essential in the design of electro-optical devices, such as solar cells. The primary aim of both theoretical and experimental investigations of silicon crystals is to elucidate the origin of visible light emission [4].

This work aims to investigate the optical dispersion parameters of silicon single crystals with different orientations on the basis of dispersion and polarization theories.

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2. Experimental

The p-silicon single crystals used in the experiments were supplied from Spectra Chemical Industries. The samples of dimensions 6 mm × 4 mm × 0.45 mm and a resistivity of 0.2 Ω·cm had (1 0 0) and (1 1 1) orientations. They were highly polished to a mirror-like surface. The transmission T (λ), at normal incidence, as well as the reflection R (λ), at an incident angle of 5°, were measured in the spectral range of λ from 200 nm to 2500 nm using a double beam spectrophotometer (JASCO, V-570 UV-Vis-NIR). The measurements were done for Si crystals with two different orientations (1 0 0) and (1 1 1). The experimental error for measured T and R was taken as ±1.5 % and for optical constants (n and k) as ±2.5 %.

3. Results and discussion

Fig. 1 presents the spectral distribution of transmittance T (λ) and reflectance R (λ) for Si crystals with (1 0 0) and (1 11) orientations, in the spectral range of 200 nm to 2500 nm. It shows that the spectral distribution of transmittance for Si crystals has strong absorption at λ ≈ 1000 nm. However, the spectral distribution of reflectance for Si crystals is

characterized by sharp structures at $\lambda < 1000$ nm, which are associated with high energy transitions from the valence band to conduction band. At $\lambda >$ 1000 nm, the reflectance decreases with increasing the wavelength.

The transmittance and reflectance values were used to calculate the absorption coefficient α according to the following equation [5–7]:

$$\alpha = (1/d)\ln\{(1-R)^2/2T + [((1-R)^4/4T^2) + R^2]^{1/2}\} \quad (1)$$

where the sample thickness is d in cm. The variation of the absorption coefficient α as a function of incident photon energy hν is shown in Fig. 2.

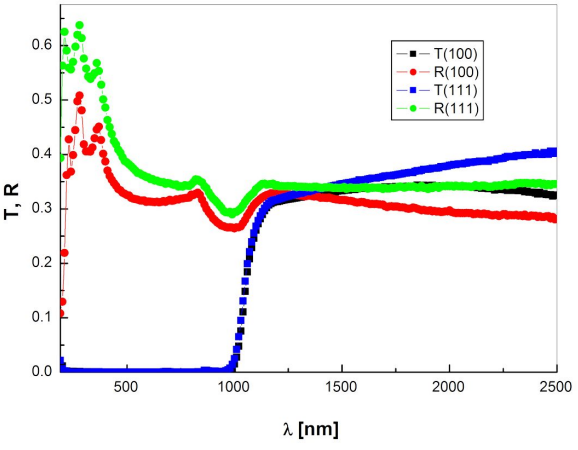

Fig. 1. Spectral distributions of transmittance, T, and reflectance, R, for Si single crystals.

The inset of Fig. 2 shows the photon energy dependence of extinction coefficient k, where $k = \alpha\lambda/4\pi$. The value of α rises with increasing photon energy for Si crystals with (1 0 0) and (1 1 1) orientations.

The dependence of absorption coefficient on photon energy was studied to get information about the optical energy gap. The relation between α and hν is given as [8, 9]:

$$(\alpha h\nu) = Y(h\nu - E_g)^p \quad (2)$$

where Y is a constant, E_g is the optical energy gap and p is an index that describes the optical absorption process. The parameter p has the values of 2,

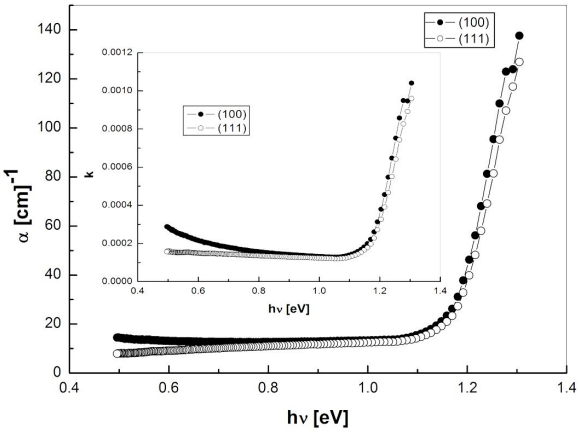

Fig. 2. Variation of absorption coefficient α, against the photon energy hν; the inset figure shows the dependence of extinction coefficient k, on the photon energy for Si single crystal.

3, 1/2 and 3/2 for indirect allowed, indirect forbidden, direct allowed and direct forbidden transitions, respectively. The plot of $(\alpha h\nu)^{1/2}$ against hν gives the best fit linear relation in the absorption region near the absorption edge, as shown in Fig. 3. The figure satisfies the equation [8]:

$$(\alpha h\nu)^{1/2} = Y(h\nu - E_g^{ind} \pm E_{ph}) \quad (3)$$

where E_{ph} is the phonon energy. It shows that the absorption takes place through the indirect allowed transition. The value of E_g is about 1.1 ± 0.025 eV for Si crystals. Thus, it is independent of the orientation. The phonon energy associated with the indirect transition was found to be ∼21.12 meV and 15.11 meV for Si crystals with (1 0 0) and (1 1 1) orientations, respectively.

The spectral distribution of the refractive index (n) was determined from the reflectance R and the extinction coefficient (k) values at the same wavelength using the following relation [10]:

$$n = [(1+R)/(1-R)] + [(4R/(1-R)^2) - k^2]^{1/2} \quad (4)$$

The refractive index n is shown in Fig. 4 as a function of hν. The spectral behavior of n shows an anomalous dispersion at photon energy >1.1 eV, which is characterized by the existence of several peaks at different energies, which are tabulated in Table 1 for different orientations. These peaks may

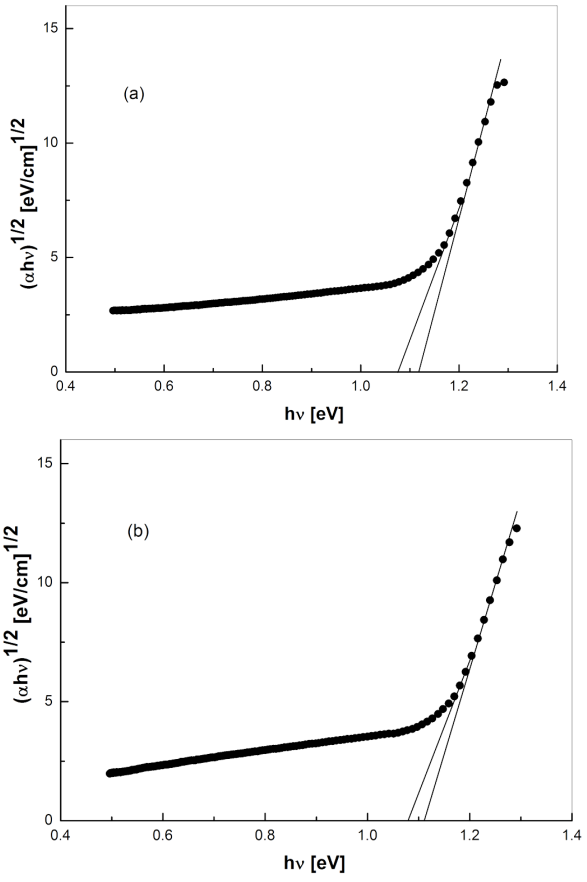

Fig. 3. Plot of $(\alpha h\nu)^{1/2}$ against the photon energy $h\nu$: (a) for Si (1 0 0), and (b) for Si (1 1 1) single crystals.

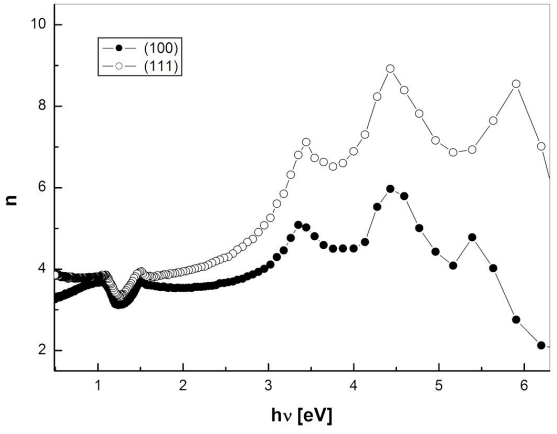

Fig. 4. The photon energy dependence of the refractive index n for Si single crystals.

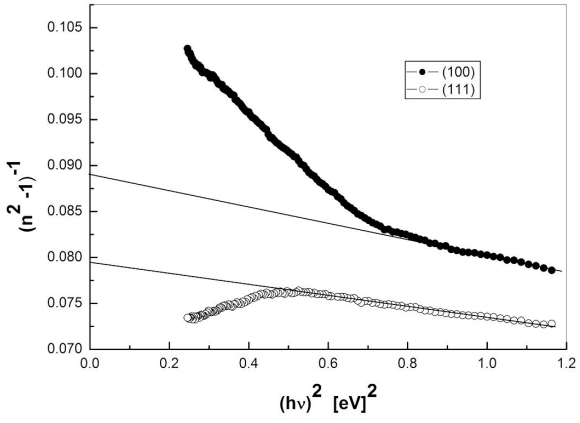

Fig. 5. Plot of $(n^2 - 1)^{-1}$ against $(h\nu)^2$ for Si single crystals.

be attributed to the band structure of the material [12]. Also, the refractive index shows a normal dispersion behavior at photon energy <1.1 eV.

Table 1. Interband transition corresponding to peak positions in the refractive index spectrum for Si single crystals with different orientations.

Orientation	Transitions [11]		
	$\Gamma_{25'} - \Gamma_{15}$	$X_4 - X_{1c}$	$L_{3'} - L_3$
(1 0 0)	3.35	4.43	5.31
(1 1 1)	3.44	4.43	5.91
Si [11]	3.43	4.4	5.5

The energy dependence of the refractive index n in the normal dispersion region can be analyzed according to the single oscillator model proposed by Wemple-DiDomenico [13, 14]. The refractive index is related to photon energy according to the relation:

$$(n^2 - 1)^{-1} = (E_o/E_d) - (1/E_oE_d) \cdot (h\nu)^2 \qquad (5)$$

where E_o is the oscillator energy and E_d is the dispersion energy. The dispersion parameters were determined by plotting $(n^2–1)^{-1}$ against $(h\nu)^2$ as shown in Fig. 5 for Si crystals of different orientations. The refractive index n(0) at zero photon energy, which is defined by the high frequency dielectric constant ϵ_∞, was deduced from the dispersion relationship by extension the linear portion like in Fig. 5. The values of E_o, E_d and ϵ_∞ were calculated and recorded in Table 2.

Table 2. Optical parameters of Si crystals with different orientations.

Orientation	E_{ph} [meV]	E_o [eV]	E_d [eV]	ϵ_∞	ϵ_L	N/m* [$cm^{-3}\cdot g^{-1}$]
(100)	21.12	3.33	37.48	12.24	12.9	4.64×10^{47}
(111)	15.11	3.66	46.13	13.59	14.61	1.53×10^{47}

An important contribution of the Wemple-DiDomenico model is interpretation of dispersion energy in terms of the chemical bonding. The dispersion energy E_d is related to other physical parameters of material by the following empirical relationship [12, 15]:

$$E_d = \beta \cdot N_c \cdot Z_a \cdot N_e \qquad (6)$$

where N_e is the effective number of valence electrons per anion, N_c is the effective coordination number of the cation nearest neighbor to the anion and Z_a is the formal chemical valence of the anion. The parameter β has two values; the ionic value $\beta_i = 0.26 \pm 0.03$ eV and covalent value $\beta_c = 0.37 \pm 0.04$ eV. β was calculated as 0.30 and 0.36 for Si crystals with (1 0 0) and (1 1 1) orientations, respectively. It indicates that the material has a covalent structure.

The refractive index n is expressed as a function of the wavelength λ by the following relation [16]:

$$n^2 = \varepsilon_L - (e^2/\pi c^2) \cdot (N/m^*) \cdot \lambda^2 \qquad (7)$$

where N/m^* is the ratio of carrier concentration to its effective mass and ϵ_L is the lattice dielectric constant. The plot of n^2 versus λ^2 is linear at longer wavelength as illustrates Fig. 6. This behavior is due to the contribution of free carriers absorption and lattice vibration modes of dispersion [12]. The extrapolation of the linear part of the plot n^2 versus λ^2 to $\lambda^2 = 0$ yields the value of the lattice dielectric constant ϵ_L, which varies from 12.9 to 14.61 depending on the crystal orientation. The N/m^* ratio was determined using the slope of the linear part of the plots in Fig. 6 and tabulated in Table 2.

Another parameter can be deduced from the refractive index behavior according to the Clausius-Mossotti model. This model introduces physically the electronic polarizability (α_e) by reducing

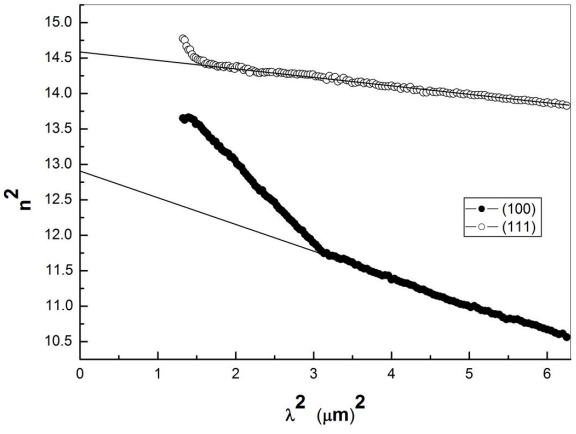

Fig. 6. Plot of n^2 versus λ^2 for Si single crystals.

the model to the well-known Lorentz-Lorenz formula [12]. The Lorentz-Lorenz relation is written as [12, 17]:

$$(n^2-1)/(n^2+2) = (N_A\rho/3M\varepsilon_o) \cdot \alpha_e \qquad (8)$$

where N_A is the Avogadro number, ρ is the mass density, M is the molecular weight of the material and ϵ_o is the permittivity of the free space. The photon energy dependence of $(n^2 - 1)/(n^2 + 2)$ for Si crystals with (1 0 0) and (1 1 1) orientations is shown in Fig. 7. From the extrapolation and equation 8, the electronic polarizability α_e was determined to be 3.84×10^{-40} Fm^2 and 4.38×10^{-40} Fm^2 at $h\nu = 0$ for Si (1 0 0) and Si(1 1 1) orientations, respectively.

On the other hand, the real and imaginary parts of dielectric constant of Si crystals were also estimated by knowing the values of the refractive index and extinction coefficient. The real and imaginary parts of complex dielectric constant are expressed as [18]:

$$\varepsilon_1 = n^2 - k^2, \quad \varepsilon_2 = 2nk \qquad (9)$$

where ϵ_1 is the real part and ϵ_2 is the imaginary part of complex dielectric constant.

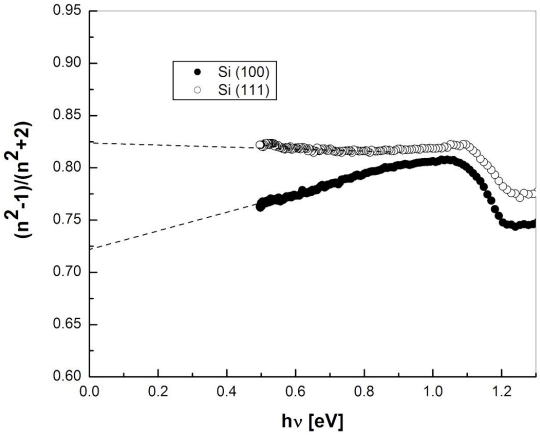

Fig. 7. Variation of $(n^2 - 1)/(n^2 + 2)$ with hν for Si single crystals.

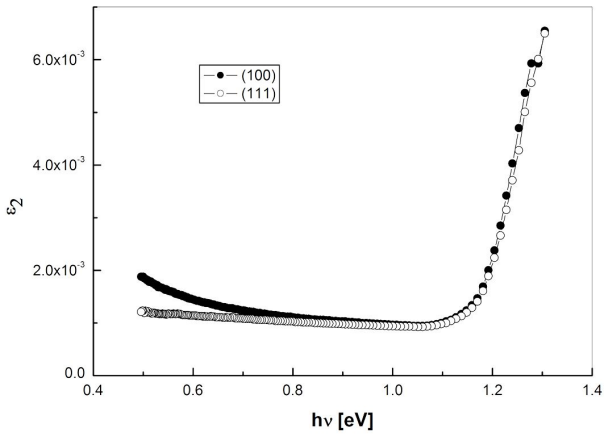

Fig. 9. Variation of ϵ_2 as a function of hν for Si single crystals.

The dependences of ϵ_1 and ϵ_2 on photon energy are shown in Fig. 8 and Fig. 9.

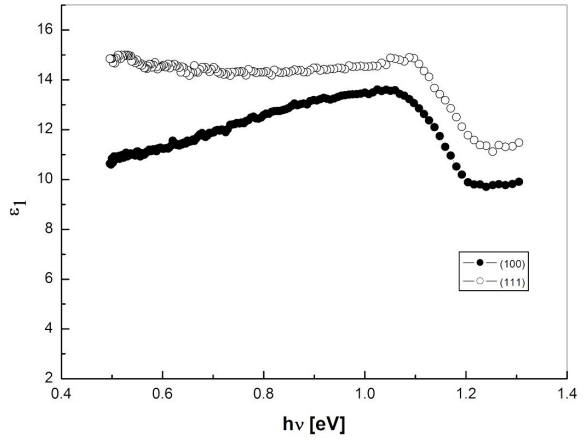

Fig. 8. Variation of ϵ_1 as a function of hν for Si single crystals.

4. Conclusions

The optical properties of Si single crystals with two orientations (1 0 0) and (1 1 1) were studied using transmittance and reflectane measurements in the spectral range of 200 nm to 2500 nm. The optical absorption data revealed the existence of indirect allowed transition band with energy gap of 1.1±0.025 eV. On the basis of Wemple and DiDomenico single oscillator model, the parameters such as of E_o, E_d, ϵ_∞, ϵ_L and β-factor were evalauted. The electronic polarizability α_e was determined for the different orientations and it was found to be 3.84×10^{-40} Fm^2 and 4.38×10^{-40} Fm^2 at $h\nu = 0$ for Si (1 0 0) and Si (1 1 1) orientations, respectively. The dependence of the real and imaginary parts of dielectric constant on photon energy was also investigated.

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