

Optical properties of phosphorus-doped polycrystalline silicon layers

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The index of refraction and the absorption coefficient of low-pressure chemical vapor deposited polycrystalline silicon (poly Si) implanted with various doses of phosphorus were obtained by means of transmittance and reflectance measurements. The refractive index of poly Si is relatively insensitive to doping in the visible region of the spectrum and agrees quite well with published values for single-crystal Si. The absorption coefficient of these films decreases with doping in the visible. Nevertheless, the absorption coefficient corresponding to the highest-doped film ($N \approx 3 \times 10^{20}/\text{cm}^3$) is almost twice the published values for lightly doped single-crystal Si. In the infrared, the index of refraction decreases systematically and the absorption coefficient increases systematically with doping. This dependence of the optical parameters on doping is attributed to the presence of free carriers. A free-carrier dispersion/absorption model is applied to the measured refractive index in the region 1.2–1.8 μm and to the reflectance measurements in the region 2.5–7.5 μm . The model gives carrier concentrations for the two types of measurements which differ by 50%. Possible explanations for this difference are discussed. The carrier concentrations and mobilities obtained from optical and Hall-effect measurements are compared.

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I. INTRODUCTION

Heavily doped ($\approx 10^{20}/\text{cm}^3$) polycrystalline silicon (poly Si) layers are often used as transparent electrodes in metal-oxide-semiconductor (MOS) imaging arrays.¹ Since the optical transmission of such layers determines the spectral quantum efficiency of these devices, it is of interest to determine the index of refraction n , and the absorption coefficient α as functions of wavelength.² The active area of a MOS photosensing device is usually covered with a multilayer structure, doped poly Si being one of the layers.

A number of papers in the literature deal with the modeling of the transmittance of such multilayer structures.^{3–6} In these papers, the index of refraction and the absorption coefficient of single-crystal Si are used in the computations.^{7–9} Kuhl, Schlotterer, and Schwidersky have shown that in particular the extinction coefficient of single-crystal Si is significantly different from that of undoped poly Si.¹⁰ In a previous publication,¹¹ the index of refraction and the absorption coefficient of poly Si, undoped and doped with phosphorus atoms to $2.9 \times 10^{20}/\text{cm}^3$, were determined in the range 0.4–0.75 μm . Using these optical constants, we calculated the transmittance of a four-phase charge-coupled device. The calculated transmittance agreed quite accurately with the experimental measurements.¹¹

In this paper we measured the optical constants of low-pressure chemical vapor deposited (LPCVD) poly Si in the range of 0.4–1.8 μm with doping density as parameter. The optical parameters of poly Si varied systematically with phosphorus doping. The index of refraction of these films has been determined by means of the interference extrema of both transmittance and reflectance measurements. Measurement of the minimum in transmittance in the infrared allowed the determination of the index of refraction and the thickness¹² of the undoped poly Si layer where absorption is negligible, as discussed in Sec. III. A new method using contours of constant $T_{\min}$ and contours of constant

$T_{\min} + R_{\max}$ is introduced, which allows the determination of the index of refraction and the extinction coefficient of doped layers where absorption is present. The thickness of the poly Si layers is then obtained from the interference condition.

The dependence of the absorption coefficient on wavelength was obtained from a numerical fit of transmittance measurements by use of the matrix method of Heavens.¹³ (Scattering of light in these films is negligible in the wavelength range of interest.) The systematic changes in the index of refraction and in the absorption coefficient with doping in the near infrared are attributed to free-carrier interaction with the radiation. Mishima, Hirose, and Osaka¹⁴ have estimated the index of refraction for heavily doped poly Si near the band-gap energy. Their index values show little dispersion and are assumed constant for wavelengths larger than 1.2 μm . Their results do not agree with our data. Dispersion in the index of refraction is expected in the infrared for heavily doped poly Si films as a result of the presence of free carriers.

A free-carrier model is used in the 1.2–1.8 μm region. A linear relationship between n_1^2 and λ^2 predicted by the model is verified experimentally. The slope of this curve yields the carrier concentration, and the extrapolation to the n_1^2 axis gives the index of refraction of the undoped poly Si. The application of the same free-carrier model to obtain a numerical fit to the measured reflectance of these layers in the 2.5–7.5 μm range gave a 50% lower carrier concentration, suggesting that the free-carrier model is not a complete description of these heavily doped layers.

II. EXPERIMENTAL PROCEDURES

A. Sample preparation

The preparation of the poly Si layers for our optical studies is schematically shown in Fig. 1. Poly Si layers were deposited on both sides of fused-quartz (SiO_2) substrates in an LPCVD system by decomposition of silane gas at 620 °C.

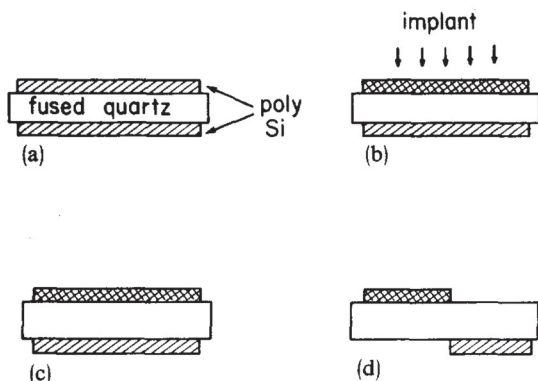


FIG. 1. Preparation of poly Si layers for optical studies. (a) Deposit LPCVD poly Si on both sides of a fused-quartz wafer. (b) Phosphorus implant one side. (c) Anneal 950 °C, 30 min in N_2 . (d) Pattern poly Si on both sides of wafer.

The substrates were polished and cleaned quartz wafers 3 in. in diameter and 0.020 in. thick. Subsequently, the poly Si film was implanted with 150-keV phosphorus, resulting in $\approx 90\%$ incorporation in the poly Si layer. Implant doses of 1×10^{15} , 5×10^{15} , 1×10^{16} , and $2 \times 10^{16}/\text{cm}^2$ were used. Both the implanted and the unimplanted samples were annealed at 950 °C in nitrogen for 30 min, resulting in a nearly homogeneous doping distribution. Finally, a pattern was etched in the poly Si on both sides of the substrate [Fig. 1(d)]. Since only one side was implanted, we have a doped and an undoped poly Si layer of equal thickness on each substrate. The resulting poly Si layers are smooth and uniformly 0.27 μm thick. The thickness of the undoped layers was accurately determined from a measurement of the minimum in transmittance in the infrared, as discussed in Sec. III. The thickness was independently measured, with excellent agreement, by a method which involved the motion of a mechanical stylus over a step in the poly Si layer.

B. Reflectance and transmittance measurements

Optical transmittance and reflectance spectra were obtained on all poly Si films. In all cases the light was incident on the poly Si film. Several instruments were used to cover the range 0.4–7.5 μm and to provide a check on the spectral and photometric accuracy. To obtain the thickness, the index of refraction, and the absorption coefficient of these layers, we measured specular spectra (collimated light incident, collimated transmission or reflection measured) on Cary 14RI and Cary 17D recording spectrophotometers in the region 0.4–2.0 μm . The measured transmittance and reflectance spectra at 0.4–2.0 μm are shown in Fig. 2 for undoped poly Si. The spectra of doped poly Si are similar to those shown in Fig. 2, with the extrema shifted to shorter wavelengths in the infrared. Comparison of specular and total transmittance measurements made at 0.4–2.0 μm shows that scattering in these films is negligible. To study the effect of interaction of infrared radiation with free carriers, we measured reflectance at 2.5–7.5 μm using the Beckman IR20A recording spectrophotometer. The measured reflectance of the poly Si films implanted with various doses of phosphorus is shown in Fig. 3. The reflectance is characterized by a mini-

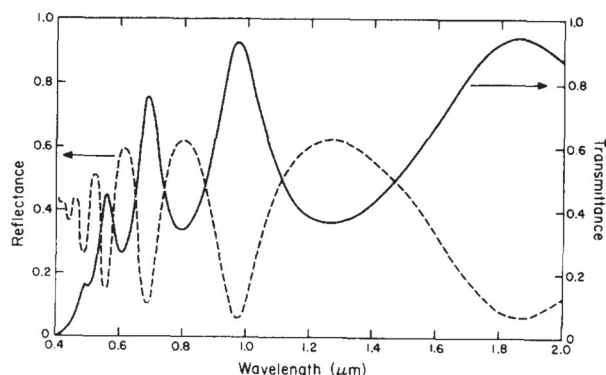


FIG. 2. Reflectance and transmittance spectra of 0.27- μm -thick, undoped poly Si layers on a fused-quartz substrate.

mum arising from free-carrier dispersion. Note that the doping in Curve A is too low for a minimum to occur in the 2.5–7.5 μm range. Reflectance measurements were not made beyond 7.5 μm because the quartz substrate shows a strong dispersion band at 9 μm .

III. THEORY

A. Matrix method—Nonabsorbing, semi-infinite substrate

The optical transmittance and reflectance of a multi-layer structure for normally incident radiation are readily calculated by a matrix method using Fresnel coefficients.¹³ Although the method is applicable to any number of layers, we will apply this method to a single layer of poly Si of thickness d_1 on a semi-infinite layer of quartz. Subsequently, in Sec. III B, the method will be modified to arrive at the calculated transmittance for our samples, which consist of a quartz substrate of finite thickness. As Fig. 4 shows, the radiation of wavelength λ is incident on the poly Si from the air side. The index of refraction of air is $N_0 = n_0 = 1$, the index of doped poly Si is complex and is given by $N_1 = n_1 - jk_1$, and the index of fused quartz is $N_2 = n_2$, a real quantity.¹⁵ The dispersion relation for n_2 given by Malitson was used.¹⁶

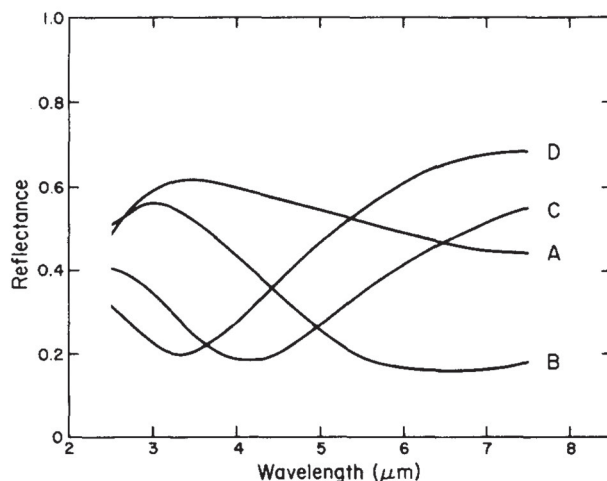


FIG. 3. Infrared reflectance spectra of 0.27- μm -thick, phosphorus-implanted poly Si layers on a quartz substrate. Implanted dose: (A) $1 \times 10^{15}/\text{cm}^2$, (B) $5 \times 10^{15}/\text{cm}^2$, (C) $1 \times 10^{16}/\text{cm}^2$, (D) $2 \times 10^{16}/\text{cm}^2$.

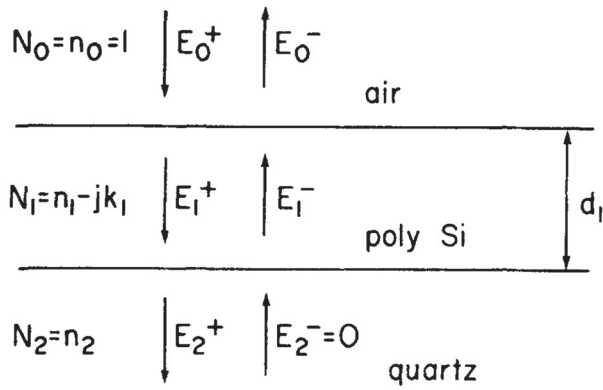


FIG. 4. Electric vectors of electromagnetic waves traveling in positive and negative directions in a layer structure consisting of a thin poly Si film of thickness d_1 on a semi-infinite quartz substrate. The radiation is incident on the poly Si film from the air side.

Experimental data of Malitson¹⁶ and Philipp¹⁷ fit this dispersion relation from 0.4 to 7.5 μm , the region of interest in this paper.

In the matrix method,¹³ the electric vectors of the positive- and negative-going electromagnetic waves in the incident medium (subscript 0) are related to those in the quartz (subscript 2) by

$$\begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} = \frac{1}{t_1 t_2} (C_1)(C_2) \begin{pmatrix} E_2^+ \\ E_2^- \end{pmatrix}, \quad (1)$$

where

$$C_m = \begin{pmatrix} e^{j\delta_{m-1}}, & r_m e^{j\delta_{m-1}} \\ r_m e^{-j\delta_{m-1}}, & e^{-j\delta_{m-1}} \end{pmatrix} \quad \text{for } m = 1, 2, \quad (2)$$

with

$$r_m = \frac{N_{m-1} - N_m}{N_{m-1} + N_m} \quad \text{for } m = 1, 2, \quad (3)$$

$$t_m = \frac{2N_{m-1}}{N_{m-1} + N_m} \quad \text{for } m = 1, 2, \quad (4)$$

and

$$\delta_{m-1} = (2\pi/\lambda) N_{m-1} d_{m-1} \quad \text{for } m = 1, 2. \quad (5)$$

Since the radiation exits in the semi-infinite quartz medium, we have no negative-going wave in this medium and $E_2^- = 0$. Furthermore, to implement these equations, we set $\delta_0 = 0$. The transmittance and reflectance of this structure can now be calculated from the relations

$$T_1 = (n_2/n_0) |E_2^+ / E_0^+|^2, \quad (6)$$

and

$$R_1 = |E_0^- / E_0^+|^2. \quad (7)$$

This formulation of the transmittance and reflectance problem was programmed in a computer with complex arithmetic capability.

B. Finite-thickness substrate

Since the quartz substrate in our samples has finite thickness, the transmittance T_1 given by Eq. (6) and the re-

flectance R_1 given by Eq. (7) do not directly predict the transmittance and reflectance of our samples. This case has been treated by Goodman.¹² His method involves expressing the total transmittance T of the sample in terms of the quantities T_1 , T_2 , R_1' , and R_2 (Fig. 5), using the assumption that the substrate thickness is sufficiently large and/or nonuniform so that light traversing it loses phase coherence and intensities can be added. Let R_1 be the reflectance at the poly Si surface and let T_1 be the transmittance into the substrate when the radiation is normally incident on the air—poly Si interface as shown in Fig. 5. Similarly, R_1' and T_1' are the comparable quantities for light normally incident on the poly Si from the substrate side. Furthermore, we let R_2 and T_2 be the reflectance and transmittance at the substrate-air interface for radiation normally incident from the substrate side.

The transmittance T can be calculated by considering the progress of a wave as it is incident on the poly Si from the air side. If I_0 is the incident intensity, $I_0 T_1$ is transmitted through the poly Si layer into the quartz substrate and $I_0 R_1$ is reflected. Since the substrate is nonabsorbing, $I_0 T_1$ is also incident on the back surface or quartz-air interface. At this surface a fraction $I_0 T_1 R_2$ is reflected and $I_0 T_1 T_2$ is transmitted. The fraction reflected becomes incident on the poly Si layer from the substrate side, and $I_0 T_1 R_2 T_1'$ is transmitted through the poly Si, becoming part of the total reflectance; $I_0 T_1 R_2 R_1'$ is reflected back into the substrate of which $I_0 T_1 R_2 R_1' T_2$ is transmitted out of the substrate, becoming part of the total transmittance.

By continuing this process, the total transmitted and reflected intensities are obtained by adding all the contributions

$$I_T = I_0 (T_1 T_2 + T_1 T_2 R_2 R_1' + T_1 T_2 R_2 R_1' R_2 R_1' \dots) \quad (8)$$

and

$$I_R = I_0 (R_1 + T_1 R_2 T_1' + T_1 R_2 R_1' R_2 T_1' + T_1 R_2 R_1' R_2 R_1' R_2 T_1' + \dots). \quad (9)$$

Summing the infinite series, we obtain

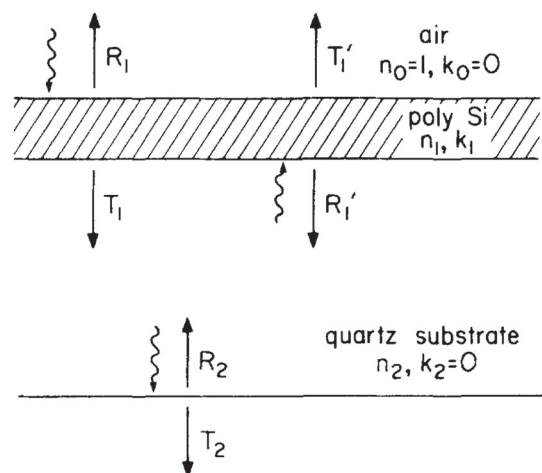


FIG. 5. Poly Si—quartz layer structure for transmittance and reflectance model. Transmittance and reflectance are considered for radiation incident at three different interfaces as shown.

$$T = [T_1 T_2 / (1 - R_1' R_2)] \quad (10)$$

and

$$R = R_1 + [T_1 T_1' R_2 / (1 - R_1' R_2)]. \quad (11)$$

The transmittance T_2 of light incident on the quartz-air interface is given by¹³

$$T_2 = 4n_0 n_2 / (n_0 + n_2)^2, \quad (12)$$

and $R_2 + T_2 = 1$. In Sec. III A, the quantities R_1 and T_1 were calculated by using a beam of light normally incident on the air—poly Si interface. Similarly, R_1' and T_1' are calculated by means of the matrix method by using a wave normally incident on the poly Si and originating in the quartz medium. Thus, the total transmittance and reflectance can be calculated for an absorbing poly Si film on a transparent substrate by means of Eqs. (10) and (11), respectively. The cases of no absorption ($k_1 = 0$) and low absorption ($k_1 \ll n_1$) are of special interest, since under these conditions the index of refraction and the thickness of the poly Si film can be determined.

1. Nonabsorbing poly Si

In the infrared, the undoped poly Si films become transparent. Under this condition $k_1 = 0$. Performing the matrix operations in Eq. (1), we obtain for the transmittance T_1 as defined by Eq. (6)

$$T_1 = (n_2/n_0) [t_1^2 t_2^2 / (1 + r_1^2 r_2^2 + 2r_1 r_2 \cos 2\delta_1)], \quad (13)$$

where r_1, r_2, t_1, t_2 , and δ_1 are given by Eqs. (3), (4), and (5). For a nonabsorbing film we also write $R_1 + T_1 = 1$, $R_1' + T_1' = 1$ (see Fig. 5). In addition, as is evident from Eq. (13), we have $T_1 = T_1'$ and thus $R_1 = R_1'$. Equation (10) can then be written as

$$T = [T_1 T_2 / (T_1 + T_2 - T_1 T_2)]. \quad (14)$$

Substituting Eq. (13) into Eq. (14) and making use of Eqs. (3) and (4), we find that the minimum of the transmittance of the poly Si—quartz substrate structure is given by

$$T_{\min} = 4n_0 n_1^2 n_2 / (n_0^2 + n_1^2)(n_1^2 + n_2^2), \quad (15)$$

which occurs when

$$2n_1 d_1 = h\lambda, \text{ where } h = 1/2, 3/2, 5/2, \dots, \quad (16)$$

under the condition that $n_0 < n_1$ and $n_2 < n_1$, which applies to our sample. A maximum in the total transmittance occurs when

$$2n_1 d_1 = (h + 1/2)\lambda. \quad (17)$$

Equation (15) is quadratic in n_1^2 , which can be solved in terms of $T_{\min}$. The refractive index of air $n_0 = 1$. Hence, a measurement of $T_{\min}$ in the infrared permits the determination of the index n_1 of the undoped poly Si layer at the wavelength under consideration. Knowledge of the approximate layer thickness establishes the order h , and thus an accurate thickness is determined from Eq. (16). Having established the thickness, the index as a function of wavelength can now be determined from the maxima and minima in transmittance. Furthermore, since a reflectance maximum coincides with a transmittance minimum and vice versa, the index can also be determined from the reflectance extrema. In fact,

reflectance extrema can be determined more accurately than transmittance extrema in the visible region of the spectrum, where the poly Si film absorbs strongly. We found that the thickness of the doped poly Si on one side of the quartz substrate is equal to that of the undoped poly Si on the other side of the substrate. This means that Eqs. (16) and (17) can also be used for determining n_1 of the doped poly Si as a function of wavelength.

When absorption takes place, analytical expressions for T_1, R_1, T_1' , and R_1' are uselessly cumbersome and numerical techniques have to be used.

2. Absorbing poly Si—contour plots

Heavily doped poly Si films will absorb radiation, even in the infrared. When undoped poly Si films are not available for thickness determination, the method of Sec. III B cannot be used to determine n_1 as a function of λ . However, when $R + T < 1$ and $k_1 \ll n_1$, the location of the transmittance minima and reflectance maxima are still accurately determined by $2n_1 d_1 = h\lambda$ with h again an odd half integer. Then d_1 is known when λ and h are determined from experiment, and n_1 is determined by means of the following procedure. Using the matrix formulation of Sec. III A, we determine $T_{\min}$ and $R_{\max}$ for sets of values n_1 and k_1 . By plotting k_1 vs n_1 , we obtain contours of constant $T_{\min}$ and contours of constant $R_{\max}$. We found it convenient to consider contours of constant $T_{\min}$ and contours of constant $T_{\min} + R_{\max}$. The point at which a contour of constant $T_{\min}$ and a contour of constant $T_{\min} + R_{\max}$ cross determines unique values of n_1 and k_1 . The intersection of the contours corresponding to the experimental values of $T_{\min}$ and $T_{\min} + R_{\max}$ then gives the desired value of n_1 and k_1 . An example of such contour plots is shown in Fig. 6, corresponding to a poly Si film implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$.

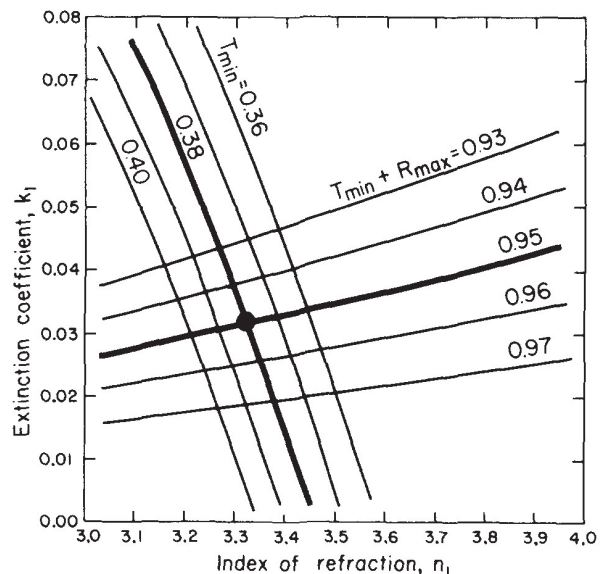


FIG. 6. Contour plots of T and $R + T$ at a transmittance minimum (reflectance maximum) with $h = 3/2$ and $\lambda = 1.20 \mu\text{m}$, corresponding to a $0.27\text{-}\mu\text{m}$ layer of poly Si implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. The heavier contours correspond to measured values of $T_{\min}$ and $T_{\min} + R_{\max}$.

C. Free-carrier absorption

The reflectance R of the poly Si film on a nonabsorbing quartz substrate can be calculated by means of the matrix method of Sec. III A. The real and imaginary parts of the complex index of refraction of the poly Si film need to be specified for this purpose. According to the classical theory of free-carrier dispersion, the real part n_1 and the imaginary part k_1 of the index of refraction can be expressed by the relations¹⁸

$$n_1^2 - k_1^2 = \epsilon_r - [\omega_p^2 \tau^2 / (1 + \omega^2 \tau^2)], \quad (18a)$$

$$2n_1 k_1 = \epsilon_i + [\omega_p^2 \tau^2 / \omega \tau (1 + \omega^2 \tau^2)], \quad (18b)$$

where ϵ_r and ϵ_i are the real and imaginary parts of the dielectric constant of the undoped poly Si, τ is the relaxation time, ω is the angular frequency of the incident radiation, and ω_p is the plasma frequency given (in MKS units) by

$$\omega_p = \sqrt{(q^2 N / \epsilon_0 m^*)}. \quad (19)$$

Here q is the magnitude of the electronic charge, N is carrier concentration, ϵ_0 is the permittivity of free space, and m^* is the effective mass of the carriers. Note that the second terms on the right-hand side of Eqs. 18(a) and (b) represent the contribution of the free carriers to the dielectric constant.

1. Wavelength region 1.2–1.8 μm

In this wavelength region, Eq. 18(a) can be simplified. The imaginary part k_1 of the refractive index, also referred to as the extinction coefficient, is related to the absorption coefficient α as

$$k_1 = \alpha \lambda / 4\pi, \quad (20)$$

where λ is the wavelength of the radiation in free space. In Sec. IV we find that $\alpha < 10^4 \text{ cm}^{-1}$ and $n_1 > 3$ in this wavelength region, so that $n_1^2 \gg k_1^2$. Furthermore, in calculating τ from the mobility (see Sec. IV), we can conclude that $\omega^2 \tau^2 \gg 1$. With these two simplifications, Eq. 18(a) can be written as

$$n_1^2 = n_{10}^2 - (\omega_p / \omega)^2, \quad (21)$$

since for undoped poly Si $\epsilon_r = n_{10}^2$, which is assumed to be constant in this wavelength region. The angular frequency can be expressed as

$$\omega = 2\pi c / \lambda, \quad (22)$$

where c is the speed of light. By means of Eqs. (19) and (22), we can now write Eq. (21) as

$$n_1^2 = n_{10}^2 - (q^2 N \lambda^2 / 4\pi^2 \epsilon_0 c^2 m^*). \quad (23)$$

Thus, a straight-line relationship is predicted between n_1^2 and λ^2 .

2. Wavelength region 2.5–7.5 μm

In this wavelength region we can set $\epsilon_i = 0$. Furthermore, we set $N = 0$ for undoped poly Si. This means that $k_1 = 0$ and $n_1^2 = n_{10}^2 = \epsilon_r$, as is evident from Eqs. 18(a) and (b). The value n_{10} is determined from experiment in Sec. IV and is assumed constant in this wavelength range. By specifying τ and N/m^* , Eqs. 18(a) and (b) can be solved simultaneously for n_1 and k_1 as a function of ω or λ . The reflectance R can then be calculated by using the matrix formulation of

Sec. III A. Variation of τ and N/m^* permits us to obtain a "best" fit of R to the measured reflectance spectrum of a given doped layer of poly Si on a quartz substrate.

IV. RESULTS AND DISCUSSION

The index of refraction as determined from the wavelength location of the reflectance of transmittance extrema is shown in Fig. 7 for the undoped and doped samples. The method outlined in Sec. III B was used. The refractive indices of lightly doped single-crystal Si measured by several authors and tabulated by Huen⁹ are shown as circles. In the visible region of the spectrum the refractive indices of the undoped and doped film are approximately equal, with the doped layer having a slightly lower index. Only the indices of refraction of the undoped (curve A) and the most heavily doped (curve E) samples are shown in the visible. The data corresponding to the intermediate doping levels fall between these curves.

The systematic variation of the index of refraction with doping in the infrared (Fig. 7) is attributed to the interaction of the radiation with free carriers. Plotting n_1^2 as a function of λ^2 results in a straight-line relationship, as predicted by Eq. (23). Such plots are shown in Fig. 8. The intercept with the n_1^2 axis gives n_{10}^2 , the square of the index of undoped poly Si, which is essentially constant in the infrared. This value agrees very well with the experimental index of 3.50 measured in the infrared (see Fig. 7, curve A). Assuming m^* is 0.28 times the mass of a free electron,¹⁹ we obtain the carrier

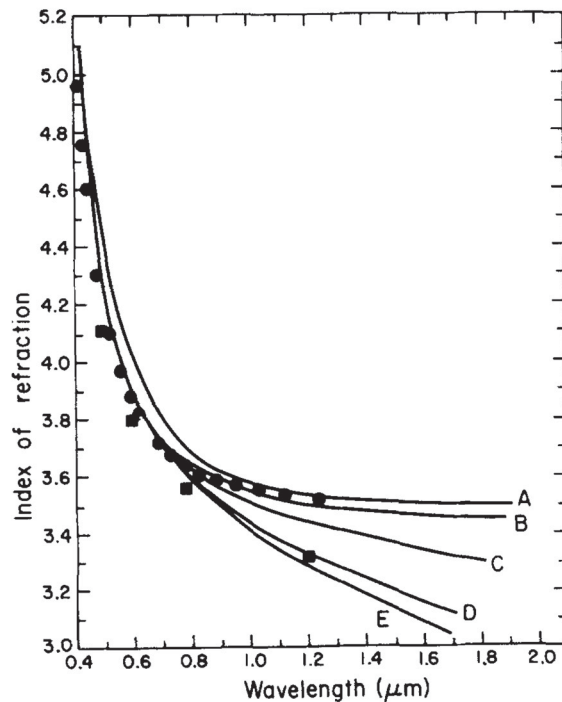


FIG. 7. Index of refraction as a function of wavelength for undoped and phosphorus-doped poly Si. Implanted dose: (A) none, (B) $1 \times 10^{13}/\text{cm}^2$, (C) $5 \times 10^{13}/\text{cm}^2$, (D) $1 \times 10^{16}/\text{cm}^2$, (E) $2 \times 10^{16}/\text{cm}^2$. The circles correspond to single-crystal Si. The squares are independently obtained from contour plots of T and $R + T$ at transmittance minima (reflectance maxima) of a poly Si film implanted with a dose of $1 \times 10^{16}/\text{cm}^2$.

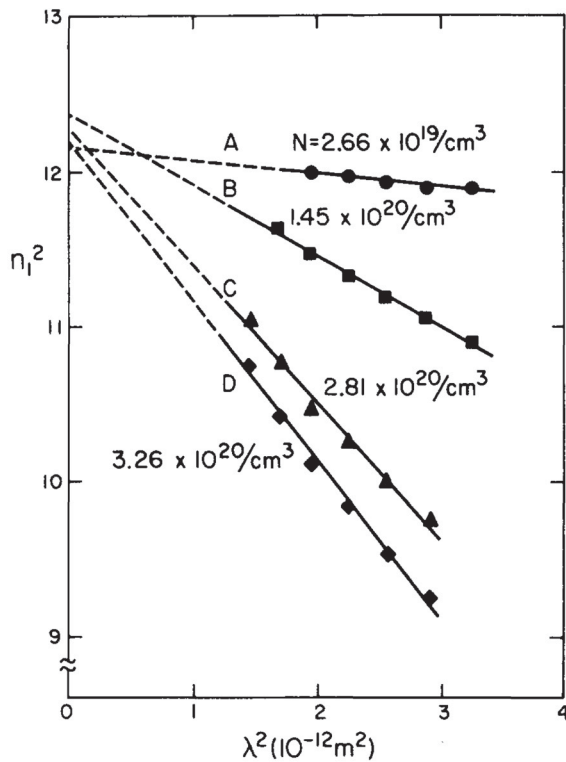


FIG. 8. Plots of n_i^2 vs λ^2 for phosphorus-implanted poly Si films. Implanted dose: (A) $1 \times 10^{15}/\text{cm}^2$, (B) $5 \times 10^{15}/\text{cm}^2$, (C) $1 \times 10^{16}/\text{cm}^2$, (D) $2 \times 10^{16}/\text{cm}^2$. The corresponding carrier concentrations N are indicated.

concentration N from the slope of the lines in Fig. 8 according to Eq. (23).

A comparison of the measured carrier concentration and the implanted dose gives the fraction of the implanted phosphorus that is electrically active. In Fig. 9 (curve A), we plot the carrier concentration of each doped poly Si layer as a function of the implanted dose of phosphorus atoms. Note that a linear relationship is obtained. However, at the highest implant doses, the carrier concentration levels off since the solid solubility is approached. From the slope of the linear portion, we find that 75% of the implanted phosphorus is electrically active.

As indicated in Sec. III C, the carrier concentration can also be deduced from the measured reflectance of these thin poly Si films on quartz substrates in the range 2.5–7.5 μm by using the same free-carrier theory. Measured reflectance curves of four doped poly Si films are shown in Fig. 3. Note that the minimum in reflectance shifts systematically to shorter wavelengths as the doping increases. This is consistent with the increase in plasma frequency with carrier density, as predicted by Eq. (19). The reflectance can be calculated by specifying τ and N , as outlined in Sec. III C. Since the mobility μ and τ are related by

$$\mu = q\tau/m^*, \quad (24)$$

we found it convenient to specify μ as defined above. Similar calculations have been reported by Lavine *et al.*, who considered the reflectance of poly Si deposited on oxidized single-crystal Si substrates.²⁰ For a "best" fit to the measured reflectance data, N and μ were varied. We found that the value

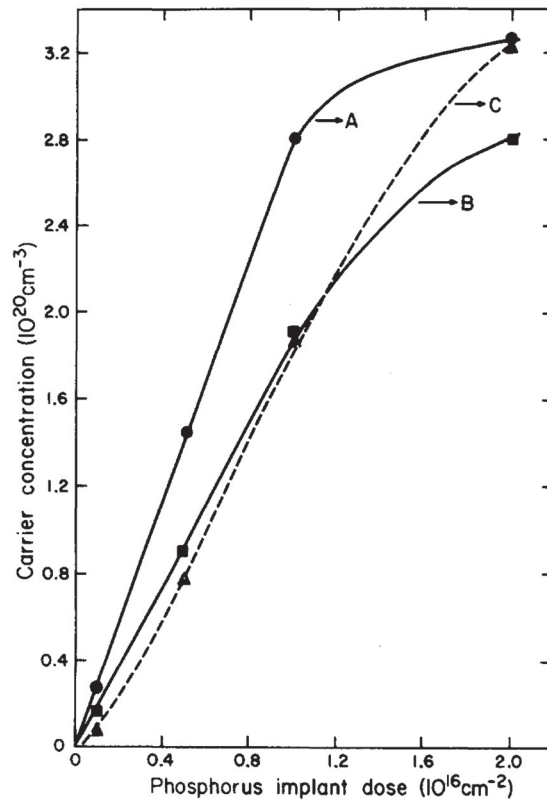


FIG. 9. Carrier concentration vs phosphorus-implant dose for 0.27- μm -thick poly Si films. A. Index of refraction analysis in the 1.2–1.8 μm region. B. Analysis of reflectance data in the 2.5–7.5 μm range. C. Hall-effect measurements.

of N primarily determines the wavelength at which the minimum in the reflectance occurs and that μ affects the shape of the curve. An example of such a calculation is shown in Fig. 10. Values of $N = 1.90 \times 10^{20}/\text{cm}^2$ and $\mu = 45 \text{ cm}^2/\text{V sec}$ were used in this calculation. Changes of 10% in either N or μ cause significant changes in the reflectance. In Fig. 9 (curve B), the values of N obtained in this manner are plotted

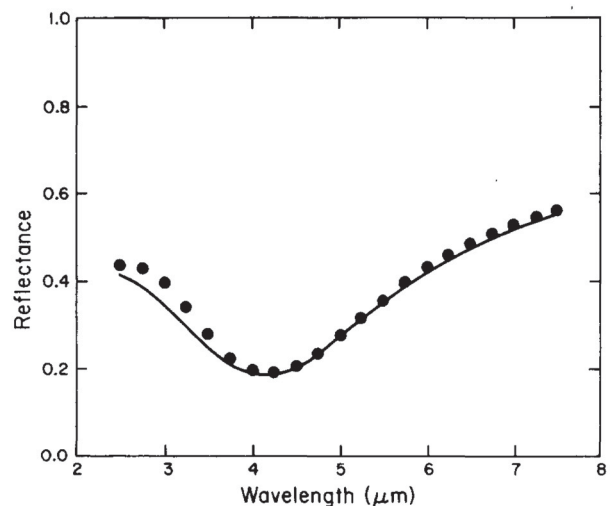


FIG. 10. Experimental (solid curve) and calculated (circles) reflectance of 0.27- μm -thick layer of poly Si on a fused quartz substrate. The sample was implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. In the calculation $N = 1.9 \times 10^{20}/\text{cm}^3$, $\mu = 45 \text{ cm}^2/\text{V sec}$, $n_{10} = 3.50$, and $m^* = 0.28$ times the free-electron mass.

for the doped samples as a function of the implanted dose of phosphorus atoms. Similar to curve A, a linear relationship is obtained at the lower implant levels. However, in this case 50% of the implanted phosphorus is electrically active as compared to the 75% electrical activity obtained previously, even though the same free-carrier theory expressed by Eqs. 18(a) and (b) is applied to the wavelength ranges of 1.2–1.8 μm and 2.5–7.5 μm .

Possible explanations for the difference between curves A and B in Fig. 9 include (1) the inadequacy of the simple free-carrier dispersion (Drude) model and (2) the occurrence of an additional optical transition which depends on the presence of free carriers. In this case, interconduction band transitions are believed to occur in heavily doped *n*-type silicon. An absorption band in the infrared is associated with these transitions.^{21–23} A refractive index change accompanies such an absorption band, and the measured index no longer is accurately described by Eqs. 18(a) and (b). Since our poly Si films are thin and the absorption in the near infrared is small, we were unable to identify an additional absorption band arising from interconduction band transitions.

After all optical measurements were completed, Hall-effect measurements using a van der Pauw pattern were made on these samples to determine the Hall mobility and carrier concentration. The carrier concentrations obtained from Hall-effect measurements are included in Fig. 9 (curve C). The carrier concentrations obtained from Hall-effect measurements compare more favorably with the carrier densities derived from reflectance measurements than with those obtained from the analysis of the index of refraction.

The mobilities obtained from fitting the reflectance data and those obtained from Hall measurements are shown in Fig. 11. The mobility derived from the Irvin curve is included for comparison. Also included are experimental Hall

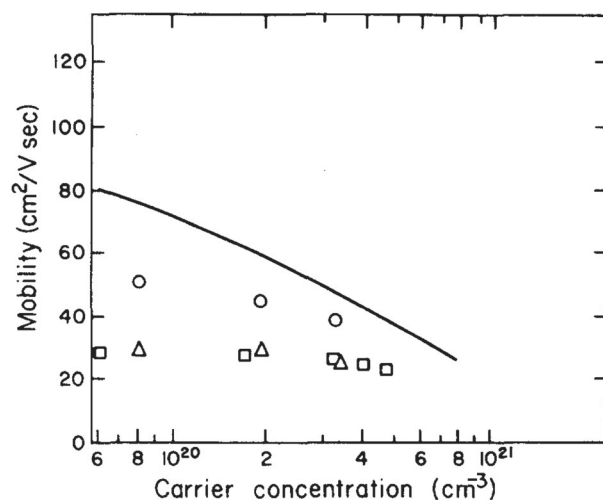


FIG. 11. Mobility of 0.27- μm -thick poly Si films as a function of carrier concentration. Δ , Hall-effect measurements; $\circ$, mobilities determined from reflectance measurements; $\square$, Hall mobilities for polysilicon as given in Ref. 24. The solid line represents single-crystal Si mobility calculated from the Irvin curve.

data reported by Shibata *et al.*²⁴ of phosphorus-implanted, 1000 °C thermally annealed poly Si layers 0.18 μm thick. The lower mobility in poly Si has been attributed to grain boundary barriers.²⁴ The Hall mobilities of our samples agree very well with those obtained by Shibata *et al.*²⁴ These data are consistent with a grain size of 0.33 μm , as determined by Shibata *et al.*²⁴

On the other hand, the mobility obtained from infrared reflectance data is a high-frequency mobility. In this case, most of the carriers are not transported across a grain boundary during a cycle of the electric field. Therefore, the reflectance mobility is expected to be larger than the Hall mobility, in agreement with observation.

The absorption coefficient α was obtained by means of a least-squares fit to the experimental transmittance. A typical fit is shown in Fig. 12 for a poly Si film implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. Other implant doses gave equally good results. The experimentally determined index of refraction and thickness of the poly Si film are used in the transmittance calculation. The transmittance can then be calculated as discussed in Sec. III B if either the extinction coefficient k_1 or α of the poly Si film is specified. We represented $\log \alpha$ by cubic splines with knots at several wavelengths.²⁵ The values of α were then determined by a nonlinear regression to give an optimum fit to the measured transmittance over the entire wavelength range of interest. As seen in Fig. 12, an excellent fit is obtained. The absorption coefficient is shown in Fig. 13 over the visible region of the spectrum for all doping levels considered.

It is seen that at the shorter wavelengths α generally decreases with doping. Nevertheless, α corresponding to the most heavily doped layer can be as much as a factor of two larger than that of lightly doped single-crystal Si. For ease of

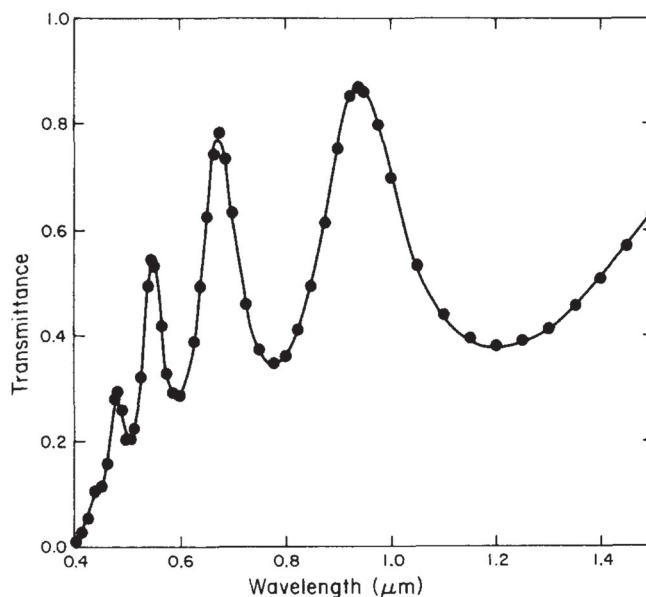


FIG. 12. Nonlinear-regression fit of the transmittance of a 0.27- μm -thick poly Si film on a quartz substrate to determine the extinction and absorption coefficients. The poly Si was implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. Solid curve: experiment. Circles: calculation.

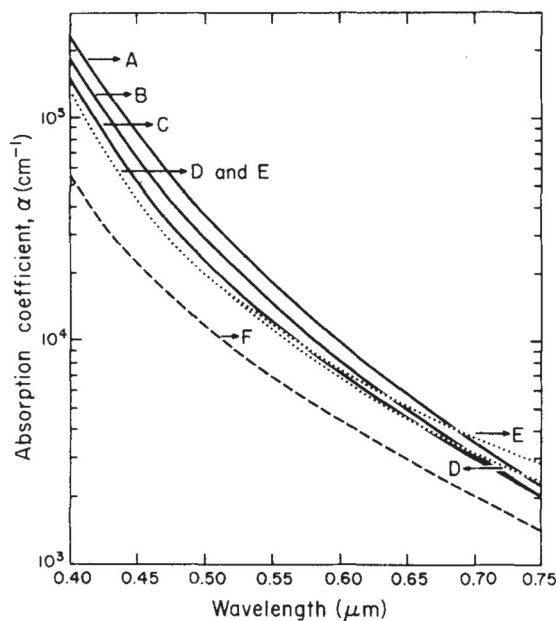


FIG. 13. Absorption coefficient of undoped and phosphorus-doped poly Si as a function of wavelength in the visible region of the spectrum. Implanted dose: (A) none, (B) $1 \times 10^{15}/\text{cm}^2$, (C) $5 \times 10^{15}/\text{cm}^2$, (D) $1 \times 10^{16}/\text{cm}^2$, (E) $2 \times 10^{16}/\text{cm}^2$. Curve F corresponds to lightly doped single-crystal Si.

reference, we give the absorption coefficient and the index of refraction in Table I for undoped poly Si and the most heavily doped (ion-implanted) poly Si film at selected wavelengths covering the visible region of the spectrum.

Figure 13 shows that at the longer wavelengths the most heavily doped films have larger α than the lower doped samples, as a result of free-carrier absorption. The effect of free-carrier absorption is further illustrated in Fig. 14, where α is plotted vs λ over the range 0.4–1.3 μm for the poly Si film implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. At 0.9 μm , α reaches a minimum and increases at longer wavelengths, owing to free-carrier absorption. As mentioned in Sec. III B, n_1 and k_1 (and therefore α) can also be determined by the method of contour plots at wavelengths corresponding to minima in transmittance without knowledge of the thickness of the layer. Contour plots similar to those shown in Fig. 6 were obtained at several transmittance minima for a poly Si film implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. The computed values of n_1 (squares in Fig. 7)

TABLE I. Absorption coefficient and index of refraction of an undoped and heavily phosphorus-doped poly Si film in the visible region of the spectrum. The doped film 0.27 μm thick was implanted with a phosphorus dose of $2 \times 10^{16}/\text{cm}^2$.

Wavelength λ (μm)	Index of refraction n_1		Absorption coefficient $\alpha (10^4 \text{ cm}^{-1})$	
	Undoped	Heavily doped	Undoped	Heavily doped
0.40	5.48	5.51	22.7	14.2
0.45	4.85	4.76	8.33	4.16
0.50	4.43	4.31	3.70	2.04
0.55	4.18	4.06	1.84	1.20
0.60	4.02	3.92	0.981	0.755
0.65	3.90	3.81	0.562	0.511
0.70	3.81	3.72	0.345	0.370
0.75	3.74	3.65	0.225	0.287

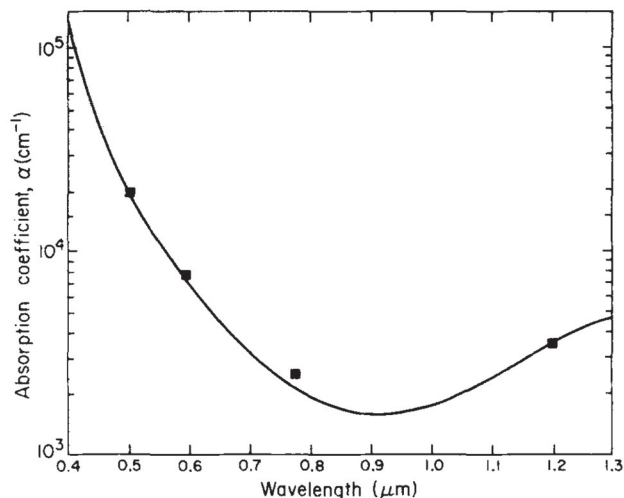


FIG. 14. Absorption coefficient as a function of wavelength in the visible and infrared regions of the spectrum for a poly Si film implanted with a phosphorus dose of $1 \times 10^{16}/\text{cm}^2$. The squares are independently obtained from contour plots.

are in good agreement with curve D. The computed values of α are shown as squares in Fig. 14. Also, in this case, the two methods are in good agreement.

V. CONCLUSIONS

The index of refraction and the absorption coefficient of undoped and phosphorus-doped poly Si films were measured in the visible and infrared regions of the spectrum. Both the index of refraction and the absorption coefficient have been tabulated for the visible region for easy reference. In the infrared, the index of refraction systematically decreases with doping and shows considerable wavelength dependence. A free-carrier absorption model explains the essential features of dispersion in the index in the 1.2–1.8 μm range. The same free-carrier model was also used to calculate the reflectance in the 2.5–7.5 μm region. The calculated and measured reflectances were in good agreement. The carrier concentrations obtained by applying the free-carrier model to both spectral regions differ by 50%. This implies that the free-carrier model is an incomplete, although useful, description of the optical behavior of heavily doped poly Si films.

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²Unless otherwise indicated, the term index of refraction will refer to the real part of the complex index of refraction.

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