Calculation of the infrared reflection spectra of inhomogeneously doped silicon semiconductor layers at an arbitrary angle of incidence

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A method is developed, based on the optical admittance, to calculate reflectance and transmittance at arbitrary angle of incidence of stratified media with arbitrary refractive index profiles. For *n*-type silicon samples, calculated and measured IR spectra are shown. In the case of a lightly doped epitaxial layer on heavily doped substrate, measurement in π polarization at the Brewster angle of the layer produces a spectrum which is free of the interference waves due to the layer and gives direct information about the profile beneath the layer. Such spectra could be used for the characterization of the transition layer between the epitaxial layer and the substrate.

I. INTRODUCTION

IR reflection spectroscopy has been applied for a long time in semiconductor research and technology for the characterization of the substrates[1,2] using the so called plasma minimum method or to measure the thickness of low-doped epitaxial layers grown on heavily doped substrates.[3-5] There were also successful attempts to characterize the diffused or ion-implanted doping profile in semiconductor structures by means of spectroscopic methods.[6-10] These methods have been based on reflection spectra measured near normal incidence.

Evaluation of the reflectance spectra involves some standard approximations concerning the optical properties of the doped semiconductor, the measurement conditions, and the doping profile. They are as follows.

A. Models for the optical properties of the doped semiconductor

The most frequently used models are Drude's model and Schumann's one. Schumann's model[11] assumes ionized impurity scattering and uses Boltzmann statistics to evaluate averages on the energy. It determines the complex permittivity of the doped silicon entirely from the dopant concentration.

Drude's model[12] is very simple. It describes the optical properties of a doped semiconductor with a two-parameter function:

$$\hat{\epsilon} = \epsilon_i\left(1 - \frac{\omega_p^2\,\tau}{\omega(\omega\tau - i)}\right), \tag{1a}$$

where the two parameters are the plasma frequency ω_p and the mean relaxation time τ. $\hat{\epsilon}$ is the complex permittivity of the doped semiconductor, ϵ_i is the same for the carrier-free one, and

$$\omega_p = \sqrt{Pq^2/\epsilon_0\epsilon_i m^*}, \tag{1b}$$

where P is the concentration of the free carriers, q is the electronic charge, m^* is the effective mass of the free carriers.

The validity of both models has been discussed by several authors. Drude's model describes the optical behavior of the doped silicon quite satisfactorily and sometimes it is better than Schumann's much more complicated model, which fails in the case of high degeneration and at low wave numbers.[13,14] In those cases when the exact connection between P and ω_p is not important, Eq. (1) can be considered as a convenient trial function in a finite wave number range with ω_p and τ as fitting parameters.

B. Approximation concerning angle of incidence

Calculating the reflectance at non-normal incidence is much more complicated than for the normal one and also the state of polarization of light has to be taken into account. Although the angle of incidence in commercial reflectance units is never exactly zero, it is customary to consider the incidence to be normal until a 30° angle of incidence as far as the reflection coefficients in silicon structures are considered. The angle of incidence is taken into account usually only in the calculation of the phase shift due to a layer. If the reflectivity cannot be measured accurately enough or if the divergence of the light beam in the spectrophotometer is comparable to the angle of incidence, this approximation is acceptable, but for higher requirements we need to know the errors this approximation may cause. On the other hand, if one has the opportunity to measure with high accuracy at arbitrary angle of incidence with polarized light, those spectra would yield a lot more information than at near-normal incidence.[15] The evaluation of the non-normal-incidence spectra requires methods to calculate the reflectance at arbitrary angle of incidence and for every state of polarization of light.

C. Approximations concerning the doping profile

The most usual approximation is to replace the profile by a step function. In those cases when the doping concentration changes by several orders of magnitude in a few

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tenths of μm it is reasonable to replace the profile by a step. It is the usual approximation when one evaluates the spectra of low-doped epitaxial layers on heavily doped substrates. This approximation makes calculations very simple and the results—the depth and the height of the concentration step—are quite sufficient in most practical cases.

The other usual procedure is to replace the profile by a stack of homogeneous layers. The main reason for this approximation is that the plane-wave formalism can be applied for such a stratified system and computer programs developed in thin layer optics can be used. This method is certainly not the best one to solve the second-order differential equations which hold for the electromagnetic field vectors or the first-order one for the optical admittance in a medium with continuously varying optical properties.

Methods have existed for a long time to treat continuous inhomogeneity in optics; they have been reviewed by Jacobsson[16] and, more recently, for transparent media by Knittl[17] using the optical admittance. However, these methods are not well known, and are rediscovered from time to time.

For weak inhomogeneities there is a well-known approximate solution: the geometric optical or WKB approximation.[18] In this solution the field vectors are composed from a traveling wave and from a reflected one as in a homogeneous layer, but these "waves" contain the exponents

$$\pm i\omega \int_0^z \sqrt{\hat{n}^2 - \sin^2 \phi_0}\, dz'$$

($\hat{n}$ is the complex refractive index and ϕ_0 is the angle of incidence), and their amplitudes also change together with $\hat{n}$. This approximation holds if the relative change of the refractive index in a wavelength is small compared to unity. In the case of stronger inhomogeneity this traveling wave-reflected wave picture loses meaning and the attempts to expand the WKB approximation to higher inhomogeneities lead to overcomplicated formulas for the reflectance,[10] often with convergence problems.[19]

The calculation of the reflectance and transmittance of inhomogeneous films can be carried out quite easily by transforming the second-order differential equations of the field vectors into first-order ones by introducing the optical admittance and then solving these first-order differential equations of Riccati's type using a standard method. Both reflectance and transmittance can be expressed in terms of the optical admittance.

In this paper, we show some calculated examples for spectra of inhomogeneously doped Si layers corresponding to various angles of incidence, and focus our attention on the Brewster-angle incidence. For illustration, we present a few measured spectra; but first, the principles will be summarized in a form which makes their use easy for semiconductor applications.

II. THEORY

A. Light propagation in inhomogeneous media in terms of the optical admittance

The electric and magnetic field vectors **E** and **H** of angular frequency ω obey the following differential equations in an inhomogeneous medium of relative permittivity $\hat{\epsilon}$ (usually a complex function) and relative permeability of $\mu = 1$

$$\Delta \mathbf{E} + (\omega^2/c^2)\hat{\epsilon}\mathbf{E} - \text{grad div } \mathbf{E} = 0, \quad (2a)$$

$$\Delta \mathbf{H} + (\omega^2/c^2)\hat{\epsilon}\mathbf{H} + (1/\epsilon)(\text{grad } \hat{\epsilon} \times \text{rot } \mathbf{H}) = 0. \quad (2b)$$

Only one-dimensional inhomogeneity will be considered:

$$\hat{\epsilon} = \hat{\epsilon}(z),$$

so we assume that the system is infinite in directions x and y; the interfaces in the system are parallel to the plane (x, y) and the inhomogeneous layer is on a homogeneous substrate of infinite thickness (Fig. 1). Let a plane wave

$$A_0 = A_0^0 \exp[i(\omega t - \mathbf{k}_0^+ \mathbf{r})]$$

be incident from the air side on the surface of the system at $z = 0$. A denotes any component of the electromagnetic field vectors **E** or **H**, $\mathbf{k}_0^+$ is the wave vector of the incident wave, and **r** is the position vector.

Assume that $\mathbf{k}_0^+$ lies in the (x, z) plane/plane of incidence. Then

$$k_{0x}^+ = (\omega/c)\sin \phi_0, \quad k_{0z}^+ = (\omega/c)\cos \phi_0, \quad (3)$$

where ϕ_0 is the angle of incidence.

As the system is homogeneous in direction x the dependence of the field vectors on x can be expressed by the factor[18]

$$\exp[-(i\omega/c)\sin \phi_0 x]. \quad (4)$$

The dependence on z will be treated separately for π polarization when the electric field is parallel to the plane of incidence and for σ polarization when the electric field is perpendicular to it. The σ polarization corresponds to the transverse electric mode TE with **E** in the y direction and the π polarization to the transverse magnetic TM mode with **H** in the y direction. The transverse field components, E_y and H_y obey the following differential equations:

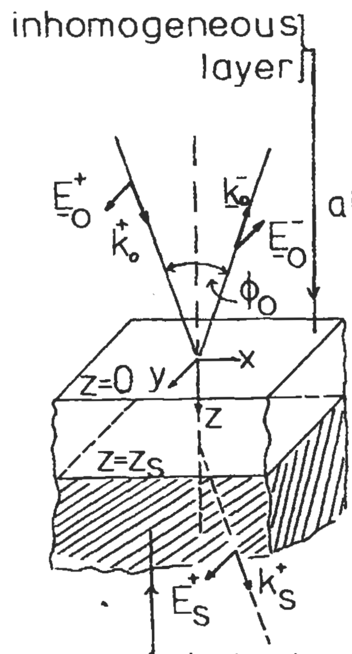

FIG. 1. Model of the inhomogeneous layer system.

$$\frac{\partial^2 E_y}{\partial z^2}+\frac{\omega^2}{c^2}(\hat{\epsilon}-\sin^2\phi_0)E_y=0\,, \tag{5a}$$

$$\frac{\partial}{\partial z}\left(\frac{1}{\hat{\epsilon}}\frac{\partial H_y}{\partial z}\right)+\frac{\omega^2}{c^2}\left(1-\frac{\sin^2\phi_0}{\hat{\epsilon}}\right)H_y=0\,. \tag{5b}$$

The parallel components can be expressed with the transversal ones according to Maxwell's equations:

$$H_x=\frac{1}{i\omega\mu_0}\frac{\partial E_y}{\partial z}\quad \text{for the transverse electric (TE) mode}, \tag{6a}$$

$$E_x=-\frac{1}{i\omega\epsilon_0\hat{\epsilon}}\frac{\partial H_y}{\partial z}\quad \text{for the transverse magnetic (TM) mode}. \tag{6b}$$

ϵ_0 and μ_0 are the permeability and permittivity of vacuum, respectively.

By definition, the optical admittance $\hat{j}$ is proportional to the ratio of the tangential field components E_t and H_t,

$$\hat{j}(z)=-\sqrt{\mu_0/\epsilon_0}\,[H_t(z)/E_t(z)]\,. \tag{7}$$

According to the boundary conditions of Maxwell's equations, H_t and E_t are continuous so $\hat{j}(z)$ is a continuous function of z in the system unless $E_t=0$.

The relations between $\hat{j}$ and the transverse field components come from Eq. (7) using Eqs. (6a) and (6b), respectively.

$$\hat{j}_{\rm TE}=\frac{ic}{\omega}\frac{\partial}{\partial z}(\ln E_y)\,;$$

$$E_y=E_y(0)\exp\left(\frac{-i\omega}{c}\int_0^z\hat{j}(z')\,dz'\right), \tag{8a}$$

$$\hat{j}_{\rm TM}^{-1}=\frac{c}{i\omega\hat{\epsilon}}\frac{\partial}{\partial z}(\ln H_y)\,;$$

$$H_y=H_y(0)\exp\left(\frac{-i\omega}{c}\int_0^z\frac{-\hat{\epsilon}(z')}{\hat{j}(z')}dz'\right). \tag{8b}$$

Substituting these expressions for E_y and H_y into Eqs. (5a) and (5b), respectively, we get the differential equations for $\hat{j}(z)$:

$$\frac{\partial\hat{j}_{\rm TE}}{\partial z}=\frac{-i\omega}{c}(\hat{\epsilon}-\sin^2\phi_0-\hat{j}^2_{\rm TE})\,, \tag{9a}$$

$$\frac{\partial\hat{j}_{\rm TM}}{\partial z}=\frac{-i\omega}{c}\left[\left(1-\frac{\sin^2\phi_0}{\hat{\epsilon}}\right)\hat{j}^2_{\rm TM}-\hat{\epsilon}\right]. \tag{9b}$$

In the homogeneous parts of the system the field is a combination of a traveling wave with spatial dependence,

$$\exp[-i(k_x x+\hat{k}_z z)]\,, \tag{10a}$$

and of a reflected one with spatial factor

$$\exp[-i(k_x x-\hat{k}_z z)]\,, \tag{10b}$$

where

$$k_x=(\omega/c)\sin\phi_0,\quad \hat{k}_z=(\omega/c)\sqrt{\hat{\epsilon}_h-\sin^2\phi_0}\,. \tag{11}$$

The optical admittance of the traveling wave in a homogeneous medium is

$$\hat{j}_{h,\rm TE}=(c/\omega)\,\hat{k}_z=\sqrt{\hat{\epsilon}_h-\sin^2\phi_0}\,,$$

$$\hat{j}_{h,\rm TM}=(-\hat{\epsilon}\omega)/c\hat{k}_z=-\hat{\epsilon}_h/\sqrt{\hat{\epsilon}_h-\sin^2\phi_0}\,. \tag{12}$$

We will call it the wave admittance and denote it by $\hat{\eta}$. So

$$\hat{j}_h=\hat{\eta} \tag{13a}$$

for the traveling wave and

$$\hat{j}_h=-\hat{\eta} \tag{13b}$$

for the reflected one.

There is only a single traveling wave in the homogeneous semi-infinite substrate so

$$\hat{j}_s(z)=\hat{\eta}_s\quad\text{for}\quad z>z_s\,,$$

and because of the continuity of $\hat{j}$,

$$\hat{j}(z_s)=\hat{\eta}_s \tag{14}$$

serves as boundary condition for the differential Eqs. (9a) and (9b).

The field in the medium where the light beam came from is the sum of the incident wave and the reflected one:

$$\mathbf{E}_0=\mathbf{E}_0^+ +\mathbf{E}_0^-\,,\quad \mathbf{H}_0=\mathbf{H}_0^+ +\mathbf{H}_0^-\,. \tag{15}$$

The reflection coefficients are defined by the ratio of the transverse components of the field vectors in the reflected wave to those in the incident wave:

$$\hat{r}_{\rm TE}=\frac{E^-_{0y}(0)}{E^+_{0y}(0)},\quad \hat{r}_{\rm TM}=-\frac{H^-_{0y}(0)}{H^+_{0y}(0)}. \tag{16}$$

There is a direct connection between the reflection coefficients and the optical admittance. For the TE mode,

$$\hat{j}(0)=-\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{H_x(0)}{E_y(0)}=-\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{H^+_{0x}(0)+H^-_{0x}(0)}{E^+_{0y}(0)+E^-_{0y}(0)}$$

$$=-\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{H^+_{0x}(0)/E^+_{0y}(0)+\hat{r}_{\rm TE}H^-_{0x}(0)/E^-_{0y}(0)}{1+\hat{r}_{\rm TE}}$$

$$=\hat{\eta}_{\rm TE}\frac{1-\hat{r}_{\rm TE}}{1+\hat{r}_{\rm TE}}. \tag{17}$$

The same formula can be derived for the TM mode. So the reflection coefficients in both modes can be obtained from the surface value of the corresponding optical admittance:

$$\hat{r}=\frac{\hat{\eta}_0-\hat{j}(0)}{\hat{\eta}_0+\hat{j}(0)}. \tag{18}$$

The power reflectance is

$$R=|\hat{r}|^2. \tag{18a}$$

With formulas (18), it is possible to calculate the reflectance of a system of arbitrary $\hat{\epsilon}(z)$ in the range $0<z<z_s$ if one knows the optical admittance at z_s and solves the differential equations (9) of $\hat{j}$ at $z=0$.

The expression for the transmittance can also be derived in terms of $\hat{j}$. Assume that the system is bounded by the same medium, air, on both sides. By definition, the transmission coefficients are

$$\hat{t}_{\rm TE}=\frac{E^+_{sy}(z_s)}{E^+_{0y}(0)};\quad \hat{t}_{\rm TM}=\frac{H^+_{sy}(z_s)}{H^+_{0y}(0)}. \tag{19}$$

Because of the continuity of the y components of the field vectors and because of Eq. (8),

$$E^{+}_{0y}(z_s) = E_y(z_s) = E_y(0)\exp\left(-\frac{i\omega}{c}\int_0^{z_s}\hat{j}(z')\,dz'\right),$$

where the subscript s refers to the substrate and the electric field in the inhomogeneous layer is denoted by E_y. According to Eqs. (15) and (16),

$$E_y(0) = E^{+}_{0y} + E^{-}_{0y} = E^{+}_{0}(1+\hat{r}_{\rm TE}),$$

so

$$\hat{t}_{\rm TE} = (1+\hat{r}_{\rm TE})\exp\left(-\frac{i\omega}{c}\int_0^{z_s}\hat{j}(z')\,dz'\right), \qquad (20a)$$

and in the same way

$$\hat{t}_{\rm TM} = (1-\hat{r}_{\rm TM})\exp\left(\frac{i\omega}{c}\int_0^{z_s}\hat{\epsilon}(z')\hat{j}^{-1}(z')\,dz'\right). \qquad (20b)$$

The power transmittance is

$$T = |\hat{t}|^2. \qquad (20c)$$

If there is a homogeneous layer in the system with boundaries z_{h_1} and z_{h_2} the field in this layer is again a combination of a traveling wave and a reflected one. The corresponding optical admittance $\hat{j}_h$ is calculated as follows inside this homogeneous part of the system:

$$\hat{j}_h = \hat{\eta}_h\left(1 - \frac{2}{1+\hat{\rho}^{-1}\exp[(2i\omega/c)\sqrt{\epsilon_h - \sin^2\phi_0}\,\Delta z]}\right), \qquad (21)$$

where

$$\hat{\rho} = \frac{\hat{\eta}_h - \hat{j}(z_{h2})}{\hat{\eta}_h + \hat{j}(z_{h2})} \qquad (21a)$$

is the reflection coefficient at the "back" boundary of the homogeneous layer and

$$\Delta z = z_{h2} - z, \quad z_{h2} > z > z_{h1}. \qquad (21b)$$

For the numerical calculations it is better to turn to real variables and to use the wave number $\tilde{\nu}$ instead of ω. Let us introduce the real variables by the following formulas:

$$\hat{j} = j_1 - ij_2, \quad \hat{\eta} = \eta_1 - i\eta_2,$$
$$\hat{\epsilon} = \epsilon_1 - i\epsilon_2, \quad \hat{\epsilon}_s = \epsilon_{s1} - i\epsilon_{s2}. \qquad (22)$$

The algorithm to calculate the reflectance of an inhomogeneous layer on a homogeneous substrate consists of solving the system of first-order differential equations

$$\frac{dj_1}{dz} = 2\pi\tilde{\nu}(-\epsilon_2 + 2j_1j_2),$$
$$\frac{dj_2}{dz} = 2\pi\tilde{\nu}(\epsilon_1 - \sin^2\phi_0 - j_1^2 + j_2^2) \qquad (23a)$$

for the TE mode and the other ones

$$\frac{dj_1}{dz} = 2\pi\tilde{\nu}\left(\epsilon_2 - 2j_1j_2 + \frac{\sin^2\phi_0}{\epsilon_1^2+\epsilon_2^2}\times[2\epsilon_1 j_1 j_2 - \epsilon_2(j_1^2 + j_2^2)]\right),$$

$$\frac{dj_2}{dz} = -2\pi\tilde{\nu}\left(\epsilon_1 - j_1^2 + j_2^2 + \frac{\sin^2\phi_0}{\epsilon_1^2+\epsilon_2^2}\times[\epsilon_1(j_1^2 - j_2^2) + 2\epsilon_2 j_1 j_2]\right) \qquad (23b)$$

for the TM modes with the boundary conditions

$$j_1(z_s) = \eta_{s1}, \quad j_2(z_s) = \eta_{s2}, \qquad (24)$$

where η_{s1} and η_{s2} are the real and imaginary parts, respectively, of the wave admittance of the substrate.

The reflectivity is obtained by the following formula:

$$R = \frac{[\eta_0 - j_1(0)]^2 + j_2^2(0)}{[\eta_0 + j_1(0)]^2 + j_2^2(0)}, \qquad (25)$$

where

$$\eta_0 = \cos\phi_0$$

for the TE mode and

$$\eta_0 = -(1/\cos\phi_0)$$

for the TM mode. η_{s1} and η_{s2} are calculated as follows. Let

$$\tilde{\epsilon}_1 = \epsilon_{s1} - \sin^2\phi_0, \quad E = \sqrt{\tilde{\epsilon}_1^2 + \epsilon_{s2}^2},$$
$$y_1 = \sqrt{0.5(\tilde{\epsilon}_1 + E)}, \quad y_2 = \sqrt{0.5(-\tilde{\epsilon}_1 + E)}, \qquad (26)$$

then

$$\eta_{s1} = y_1, \quad \eta_{s2} = y_2$$

for the TE mode and

$$\eta_{s1} = \frac{-\epsilon_{s1}y_1 - \epsilon_{s2}y_2}{E}, \quad \eta_{s2} = \frac{-\epsilon_{s2}y_1 + \epsilon_{s1}y_2}{E} \qquad (27)$$

for the TM mode.

III. CALCULATION OF THE REFLECTANCE SPECTRA OF n-TYPE SILICON LAYERS WITH SEVERAL CONCENTRATION PROFILES OF THE FREE CARRIERS

Our reflectance-calculating program has been written in ALGOL 60 for a CDC 7600 computer. The program is based on a standard Runge–Kutta procedure which calculates the surface value of the optical admittance by solving the two-variable system of differential equations (23) with the boundary conditions (24). The program also uses a procedure to calculate the optical quantities ϵ_1 and ϵ_2 along the profile and another one for the calculation of the free-carrier concentration at a given depth z. The calculations were carried out at the University College of North Wales, Bangor, Gwynedd, Wales.

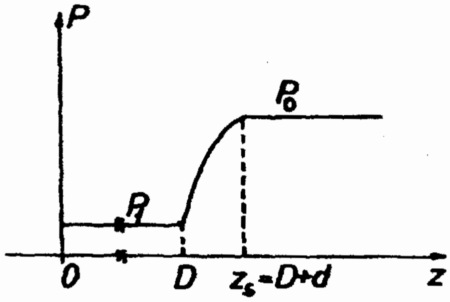

FIG. 2. Model of the Si epitaxial layer–substrate system.

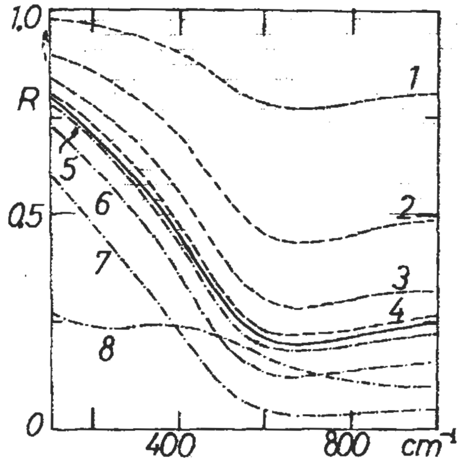

FIG. 3. $R\sigma$ and $R\pi$ spectra of an n-type homogeneous silicon substrate with $P_0 = 10^{19}\,\mathrm{cm}^{-3}$ concentration of the free carriers at different angles of incidence. Full line: normal incidence; dashed line: $R\sigma$ spectra, angles of incidence are 1–80°, 2–60°, 3–40°, 4–20°: dash-dotted line: $R\pi$ spectra, angles of incidence are 5–20°, 6–40°, 7–60°, 8–80°.

The optical variables ϵ_1 and ϵ_2 were calculated according to Drude's model (1). In real variables and in terms of the wave number they are

$$\epsilon_1 = \epsilon_i\left(1 - \frac{\tilde{\nu}_p^2}{\tilde{\nu}^2 + \tilde{\nu}_e^2}\right),$$

$$\epsilon_2 = \epsilon_i \frac{\tilde{\nu}_e}{\tilde{\nu}} \frac{\tilde{\nu}_p^2}{\tilde{\nu}^2 + \tilde{\nu}_e^2},$$

where ϵ_i is the permittivity of the carrier-free silicon, $\epsilon_i = 11.7$, $\tilde{\nu}_p$ is the plasma wave number,

$$\tilde{\nu}_p(\mathrm{cm}^{-1}) = \frac{\omega_p}{2\pi c} = \sqrt{0.7659\times 10^{-14}\,P(\mathrm{cm}^{-3})}\Big/\frac{m^*}{m_e},$$

and $\tilde{\nu}_e$ is a characteristic wave number proportional to the collision frequency $1/\tau$:

$$\tilde{\nu}_e = 1/2\pi\tau c\,.$$

We used the value $m^*/m_e = 0.26$ for the free electrons and

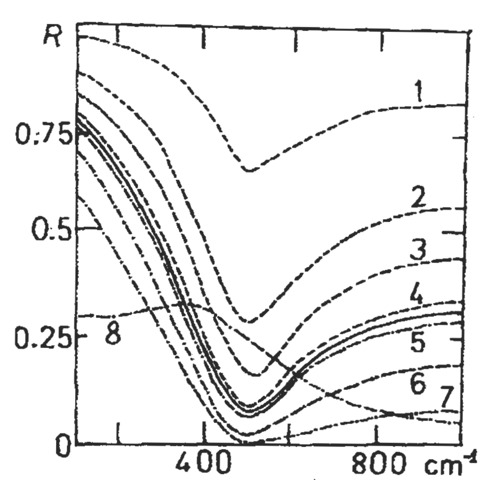

FIG. 4. $R\sigma$ and $R\pi$ spectra of a surface layer with linearly decreasing concentration of the free carriers on an n-type substrate. $P_0 = 10^{19}\,\mathrm{cm}^{-3}$, $P_1 = 10^{15}\,\mathrm{cm}^{-3}$, the thickness of the surface layer is $d = 1\,\mu$m. The notations are the same as in Fig. 3.

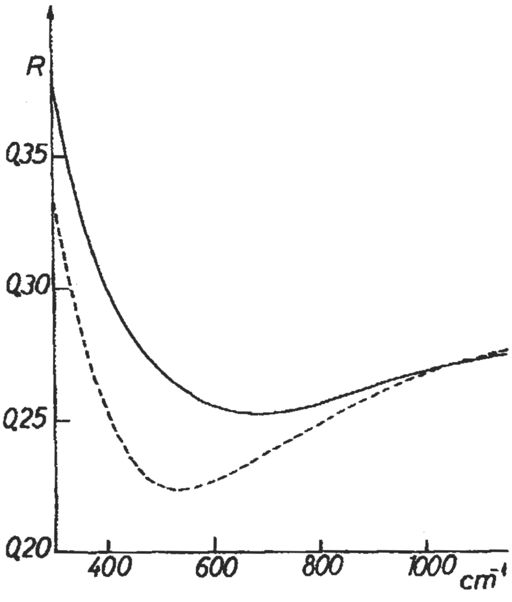

FIG. 5. Measured spectra of a boron-doped silicon substrate with and without an outdiffused layer. The spectra were measured at 6.5° angle of incidence with unpolarized light. Full line: original substrate; dashed line: spectrum after heat treatment in dry oxygen at 1050 °C for 3 h.

$\tilde{\nu}_e$ was calculated from the following experimental relationship:

$$\tilde{\nu}_e = 733.7/(1 + 627.3/\tilde{\nu}_p).$$

The calculations were carried out for systems which corresponded to a lightly doped layer on a heavily doped substrate and a transient layer between them where the concentration increased linearly from a value characteristic of the layer to that of the substrate (Fig. 2).

$$P(z) = P_1\,,\quad 0<z<D\,,$$

$$P(z) = P_1 + (P_0 - P_1)(z - D)/d\,,$$

$$D<z<D + d = z_s\,,$$

$$P(z) = P_0\,,\quad z_s<z\,.$$

The calculated spectra are presented in Figs. 3, 4, 6–8.

Spectra for homogeneous n-type silicon $P_0 = 10^{19}\,\mathrm{cm}^{-3}$ are shown for several angles of incidence in Fig. 3. It can be seen that $R\sigma + R\pi$ agrees with R_1 in that $R\sigma + R\pi$ does not differ more than 1% reflectance (0.01) if the angle of incidence is less than 20°. Note that $R\pi$ spectrum changes its shape completely if the angle of incidence exceeds the Brewster angle of silicon, $\phi_B = 73.7°$.

The spectra as shown in Fig. 3 and especially those near the Brewster angle could serve as a check of the theoretical model of the optical properties. Measuring at two angles of polarizations would provide the two parameters of the Drude model $\tilde{\nu}_p$ and $\tilde{\nu}_e$ at a given wave number, and if these parameters remain constants in a wave number range the optical model is proven to be true in that range.

Spectra in Fig. 4 are of a surface layer with linearly decreasing concentration. The concentration of the substrate is $P_0 = 10^{19}\,\mathrm{cm}^{-3}$ and it decreases to $P_1 = 10^{15}\,\mathrm{cm}^{-3}$ in $d = 1\,\mu$m. The minima of the reflection curves and the maximum of $R\pi$ at 80° angle of incidence became sharper than those for the homogeneous substrate. $R\pi$ changed shape again between 60° and 80°.

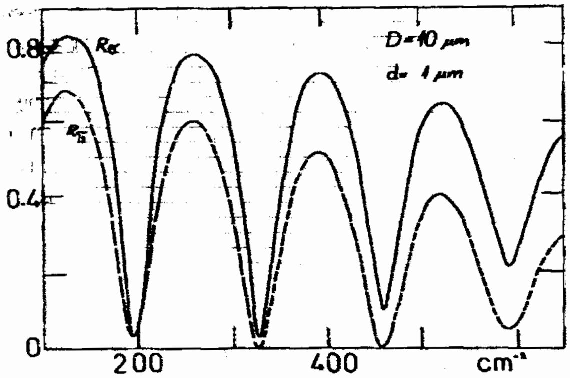

FIG. 6. 45° angle of incidence spectra $R\sigma$ (full line), $R\pi$ (dashed line) for an epitaxial layer on a heavily doped silicon substrate. Concentration in the substrate $P_0 = 10^{19}$ cm^{-3}, that in the homogeneous layer is $P_1 = 10^{15}$ cm^{-3}. The thickness of the transition layer with linear concentration profile is $d = 1$ μm.

For comparison, we show spectra in Fig. 5 measured on a boron-doped silicon substrate before and after heat treatment in oxygen at 1050 °C for 3 h. The spectra were measured at a 6.5° angle of incidence with unpolarized light. The spectrum of the heat-treated sample shows deeper minimum shifted to lower wave number compared to the original one, just as the 0° angle curves in Figs. 3 and 4 indicating that an outdiffused layer had been formed during the heat treatment. In that way, IR spectra provide a quick and nondestructive check of the homogeneity of a semiconductor sample.

In Fig. 6, $R\pi$ and $R\sigma$ spectra of the silicon epitaxial layer system are shown. The system consists of a lightly doped layer $P_1 = 10^{15}$ cm^{-3} of thickness $D = 10$ μm on a heavily doped substrate $P_0 = 10^{19}$ cm^{-3} and a transition layer of $d = 1$ μm between them with linear profile. The angle of incidence is 45°.

Figure 7 shows how the spectra of the above system

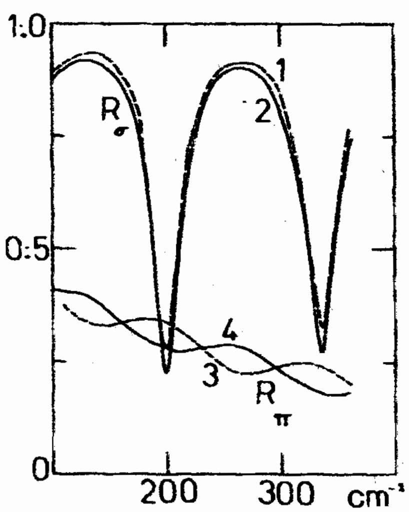

FIG. 7. $R\sigma$ and $R\pi$ spectra of the system above near the Brewster angle of the homogeneous layer, $\phi_B = 73.7°$. Full lines: $\phi_0 = 72.5°$; dashed lines: $\phi_0 = 75°$.

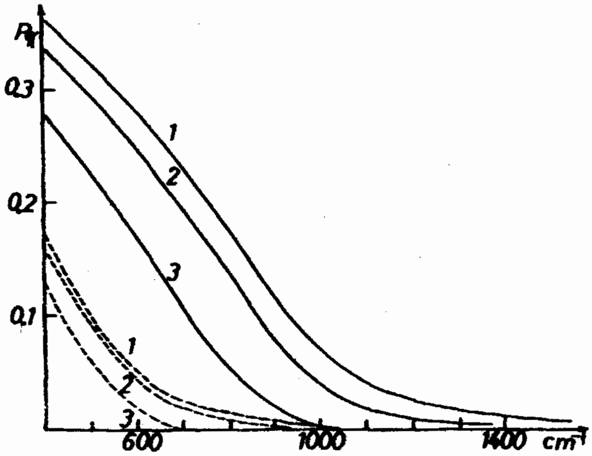

FIG. 8. $R\pi$ spectra at the Brewster angle of the epitaxial layer ϕ_B. Full line: $P_0 = 3\times10^{19}$ cm^{-3}; dashed line: $P_0 = 1\times10^{19}$ cm^{-3}. The concentration in the layer is $P_1 = 10^{15}$ cm^{-3}. The thickness of the transition layers are 1–0.5 μm, 2–1 μm, 3–2 μm.

change near the Brewster angle of the layer. The spectra were calculated for 75° and 72.5° angles of incidence. The phase of the interference pattern in the $R\pi$ spectra are reversed and the interference waves completely disappeared at the Brewster angle. As there is no reflected wave in the TM mode from the layer/air interface at ϕ_B all the reflected intensity arises from the back profile. Such spectra, without the disturbing interference waves, could provide direct information about the back profile or about the substrate beneath a homogeneous transparent surface layer.

Figure 8 shows the Brewster-angle $R\pi$ spectra of the bare transient layer for different thicknesses d and for different substrate concentrations P_0. A decrease of both the substrate concentration and the slope of the profile caused a similar effect: the spectra shifted to lower wave numbers. So it is difficult to obtain both the substrate concentration and the gradedness of the profile from the $R\pi(\phi_B)$ spectrum, but if the substrate concentration is known the gradedness can be estimated.

Figure 9 shows $R\pi(\phi_B)$ spectra measured both on the layer side and on the polished substrate side of a silicon slice with an epitaxial layer. The substrate was doped with As, the carrier concentration was 2.9×10^{19} cm^{-3} determined from the 6.5° angle of incidence reflection spectrum. The epitaxial layer was grown from $SiCl_4$ at 1100 °C, the surface free-electron concentration was about 10^{15} cm^{-3}. The spectra were measured with a Perkin-Elmer PE-580A infrared spectrophotometer, using a Perkin-Elmer variable angle specular reflectance unit and a common-beam gold wire grid polarizer. The reflectance was measured against a front surface Al reference mirror. Reflectance of the mirror was calculated from the optical constants given by Shiles.[20] In Fig. 9, calculated spectra for a homogeneous substrate with $P_0 = 3\times10^{19}$ cm^{-3} and for a substrate-linear transient layer system with parameters $P_0 = 3\times10^{19}$ cm^{-3}, $d = 2$ μm are also plotted.

The correspondence between measured and calculated spectra suggests that measuring at the Brewster angle could

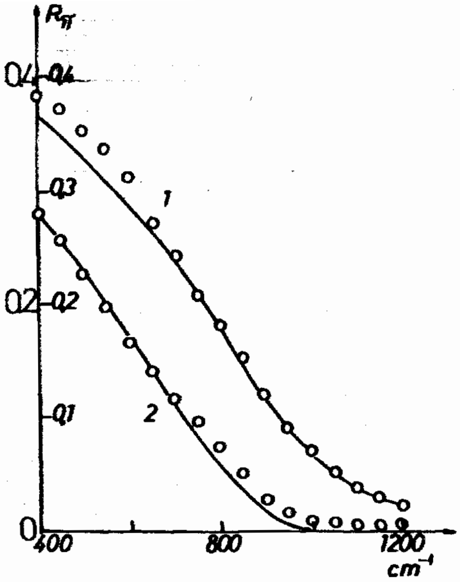

FIG. 9. Measured and calculated R_{ff} spectrum of the substrate side (1) and of the layer side (2) of a silicon slice with epitaxial layer. The measured reflectances are denoted by O. Parameters of the calculated spectra are 1—$P_0 = 3\times10^{19}$ cm^{-3}, $d = 0$; 2—$P_0 = 3\times10^{19}$ cm^{-3}, $d = 2$ μm.

be a powerful method of obtaining information about buried concentration profiles beneath transparent surface layers.

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