The effect of surface and volume imperfections upon the absorption coefficient of semiconductor sample

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The paper deals with the effect of surface and volume imperfections of the real semiconductor samples upon the results of transmittance and reflectance at normal incidence. The method is discussed to compute the absorption coefficient including the above effect and an exemplary analysis is performed of the experimental data.

1. Introduction

The semiconductor literature contains many papers dealing with determination of absorption coefficient of semiconductor sample. Usually, a perfectly uniform wafer with perfectly smooth surfaces has been assumed. However, it has become known [1–4] that the surface and volume imperfections on the microscale affect significantly optical properties of thin films of semiconductors, even microscopically uniform. The effect of surface roughness upon the sample reflectivity has been discussed recently in papers [4–7] and an attempt to include the surface roughness into determination of the absorption coefficient has been made in [6, 8].

Statistical treatment of both the surface and volume imperfections was crucial to develop the model [9] of determination of the effect of these imperfections upon the transmittance and reflectance at normal incidence. The model has been used to derive the formulae to compute the absorption coefficient for the real sample and is applied in this paper.

2. Method of calculations

Both the geometrical and physical imperfections (in the sense given in [9]) have been considered on the surface and in the volume of the sample. The geometrical imperfections give rise to the diffused light, while the physical ones characterise the additional absorption phenomena (different than those

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connected with the band-to-band transitions or any other transitions in the energy band structure we are searching for, e.g., intraband transitions and to/from impurity levels).

Surface imperfections have been included into the Fresnel amplitude coefficient reflectance (index R)·

$$\hat{r}_{ij} = \hat{r}_{ij}^0 \exp\left[-\frac{1}{2}(\hat{\Phi}_{RG\ ij}^2 + \hat{\Phi}_{RP\ ij}^2)\right],$$

and transmittance (index T)   (1)

$$\hat{t}_{ij} = \hat{t}_{ij}^0 \exp\left[-\frac{1}{2}(\hat{\Phi}_{TG\ ij}^2 + \hat{\Phi}_{TP\ ij}^2)\right]$$

where the second subscript, G or P, denotes that the phase shift is caused by the geometrical or physical imperfections, respectively, and $\hat{r}_{ij}^0$ and $\hat{t}_{ij}^0$ are the Fresnel coefficients of the ideal surface/interface.

Volume imperfections have been included into the phase thickness $\hat{\tau}$ of the sample

$$\hat{\tau} = \hat{\beta} + \hat{\gamma}$$ (2)

where

$$\hat{\beta} = \frac{2\pi}{\lambda}(n - ik)d$$ (3)

is a phase thickness of the ideal wafer with geometrical thickness d and complex refractive index $\hat{N} = n - ik$, and

$$\hat{\gamma} = \frac{2\pi}{\lambda}(\eta - i\varkappa)d.$$ (4)

Here η is ascribed to the geometrical imperfections and $\varkappa$ to the physical ones, both being the result of fluctuation of the complex dielectric permittivity.

In practice, semiconductor samples are highly absorbing near to and above the fundamental absorption edge (FAE), thus multiple reflections can be neglected. Also, these wafers are usually measured in air ($n \cong 1$, $k \cong 0$) and
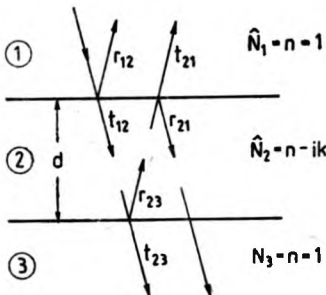

Fig. 1. Schematic representation of a semiconductor sample surrounded by semi-infinite media 1 and 3

without any supporting substrates. The configuration of semiconductor wafer surrounded by semi-infinite media is shown in Fig. 1. The amplitude coefficients of reflectance and transmittance are then given by

$$\hat{r} = \hat{r}_{12} \text{ and } \hat{t} = \hat{t}_{12}\hat{t}_{23}\exp(-i\tau), \tag{5}$$

respectively, and the power Fresnel coefficient by

$$R = R_{12}^0 \exp(-L_{RG\,12}^2 - L_{RP\,12}^2), \tag{6a}$$

$$T = (1-R_{12}^0)(1-R_{23}^0)\exp(-L_{TG\,12}^2 - L_{TG\,23}^2 - L_{TP\,12}^2 - L_{TP\,23}^2)\exp(-a_r d - a_{im}d) \tag{6b}$$

where R_{12}^0 and R_{23}^0 are power coefficients of the ideal surfaces of the sample, terms $L_{\alpha\beta ij}^2$ are the real parts of $\hat{\Phi}_{\alpha\beta ij}^2$, respectively, $a_r = 4\pi k/\lambda$, and $a_{im} = 4\pi\varkappa/\lambda$. Equation (6b) can be rewritten as

$$a_r d + a_{im} d + A_S = \ln \frac{(1-R_{12}^0)(1-R_{23}^0)}{T} \tag{7}$$

where A_S is a sum of the terms $L_{TG,TP,12,13}^2$. The first term of Eq. (7) means true/real absorption of the material, the second term describes the absorption on volume imperfections, and the third one characterises optical losses (artificial absorption) on surface imperfections, which can be partially accounted for in the measuring systems equipped with integrating sphere. The second and the third terms in Eq. (7) constitute the background absorption (BA) found always in experiments. Note that only term $a_{im}d$ is thickness-dependent and dominates over term A_S in a thick sample, while A_S prevails in very thin films; provided that the other conditions are the same and typical of semiconductor sample.

The function of $a_{im}(\hbar\omega)$ is generally unknown and results from many possible processes [9] which can have quite different energy spectra. Term A_S is proportional to $\hbar\omega$ and also reflects the energy dependence of refractive index of semiconductor. Although the energy dependence of the BA is not known precisely, we have assumed that it has not any singularity in the region of the FAE. Therefore, taking the data of R and T measured below the FAE and assuming that there $a_r = 0$, we find the shape of the energy dependence of the BA. Next, this dependence is extrapolated into the region of the FAE and slightly above it, and therefore $a_r(\hbar\omega)$ can be found. Furthermore, using the set of identical samples with different thicknesses, both terms of the BA, i.e., A_S and $a_{im}d$ can be estimated. This procedure is shown below taking the experimental data of $(Zn_x Cd_{1-x})_3 P_2$ mixed crystals.

3. Experimental results

Common source of information about absorption coefficient is the energy spectrum of reflectivity and transmittivity at normal incidence. It provides with the data to compute the right side of Eq. (7). Note that the value of reflectivity is affected itself by the surface imperfections and R^0 has to be determined before Eq. (7) is applied. A few methods to find R^0 can be suggested, namely: (1) by means of series of reflectivity measurements of wafers with differently prepared surfaces, from the very rough to the reasonably flat* (see e.g., experiments with Si surface [10]) followed by a careful analysis of the data [7]; (2) from the definition, i.e., from formula $R^0_{ij} = [(n_i - n_j)^2 + (k_i - k_j)^2]/[(n_i + n_j)^2 + (k_i + k_j)^2]$, assuming the reliable data of $n_{i,j}$ and $k_{i,j}$ are available, (3) by means of ellipsometry technique [11], and (4) by using the special algorithm of Kramers-Krönig analysis of the experimental data, presented recently [12].

In the case of $(Zn_x Cd_{1-x})_3 P_2$ crystals discussed below, the experimental data of R (uncorrected for surface imperfections) have been taken from [13] and [14], for Zn_3P_2 and Cd_3P_2, respectively, and R values for appropriate molar content x assumed to be linearly dependent on x and computed as $R(x) = xR(Zn_3P_2) + (1-x)R(Cd_3P_2)$. The r m.s. values of roughness, σ, have been estimated for sufraces of a few samples investigated from the measurements of the sufrace profile by means of Dektak Surface Profile Measuring System (by Sloan) and taken as equal to 20 nm in all the samples. Next, the coherent term in equation given by PORTEUS [5]

$$R = R^0 \exp\left[-\left(\frac{4\pi\sigma}{\lambda}\right)^2\right] \tag{8}$$

was used to compute R^0. This procedure shifted the experimental values of $R \rightarrow R^0$ up by a few per cent.

The preparation of the samples investigated and measuring procedure have been described elsewhere [15]. The important point was to get all the surface done in the same manner; furthermore, to get all the surfaces as identical as possible. The sample holder shown in Fig. 2 was used, and the starting sample thickness were in the region of 0.3–0.4 mm. After the first measurement run, the wafers were etched from both sides in a solution of 1 per cent bromine in methanol and then measured again. The procedure was repeated five-six times for each sample. The initial and final thicknesses were measured directly and the known etching rate was used to estimate the thickness in between, with the error not exciding 0.025 mm, approximately. This method made it possible to measure the transmittivity of the same wafer (the same a_{im})

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* r.m.s. values of roughness can be less than 5 nm when electro-polishing is applied.

at different thicknesses, with A_S maintained on the same (presumably) level throughout the measurement procedure.

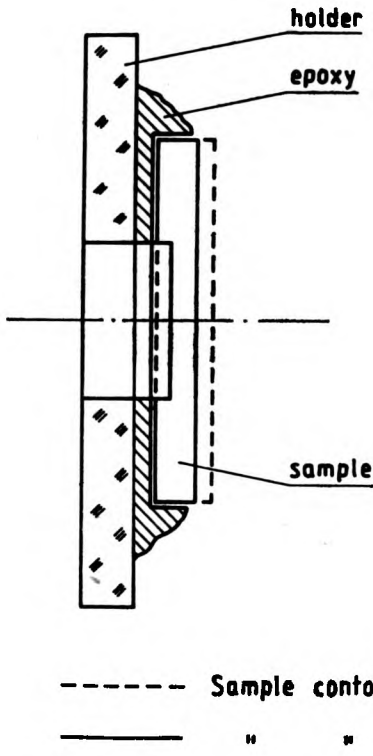--- --- --- Sample contour before etching

─────── " " after etching

Fig. 2. Sample holder used in the experiments

Exemplary results for one of the samples are shown in Fig. 3. The energy dependences of the BA (thin lines in this figure) for different thicknesses were used to compute a_{im} and A_S and their spectral dependences. The computation was done by solving each time the set of two equations (at $\hbar\omega = $ const.)

$$\begin{aligned} \text{BA}' &= a_{im}d' + A_S, \\ \text{BA}'' &= a_{im}d'' + A_S, \end{aligned} \tag{9}$$

for two different runs/thicknesses of the sample, assuming both the A_S and a_{im} unchanged. However, this requirement is easily met by a_{im} only. Results marked by points are shown in Fig. 4. The curve of A_S-versus-$\hbar\omega$ dependence resulted from the fitting procedure described below.

According to Filinski's approximation [6], the surface roughness with the r.m.s. value of σ affects the power transmittivity coefficient as follows:

$$T = T^0 \exp\left[-\left(\frac{2\pi\sigma}{\lambda}\right)^2 (n-1)^2\right]. \tag{10}$$

Hence, assuming both surfaces of the sample to be identical,

$$L^2_{TG\ 12} = L^2_{TG\ 23} = \left[\frac{2\pi\sigma}{\lambda}(n-1)\right]^2, \tag{11}$$
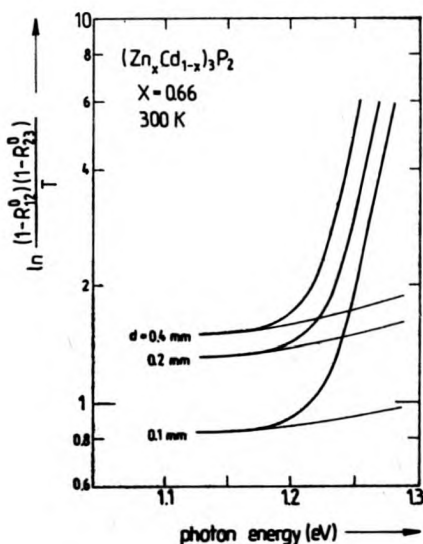

Fig. 3. Experimental results of total absorptivity versus energy (thick lines) and background absorption (thin lines)
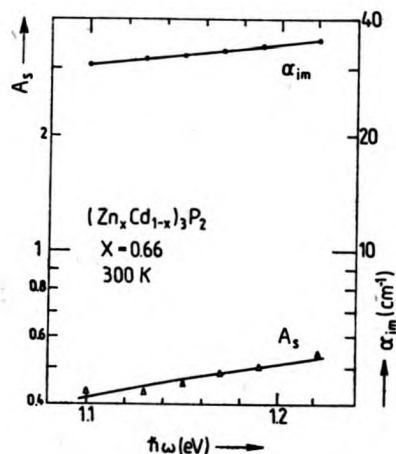

Fig. 4. Optical losses on the surface, A_S, and the coefficient of absorption on volume imperfections, a_{im}, estimated from the BA spectra

and $L^2_{TP} \leqslant L^2_{TG}$, one can fit the theoretical curve $A_S = 2L^2_{TG\ 12}$ from Eq. (11) to the experimental data by using σ as the fitting parameter. That was done for the samples measured and the values of σ in the range of 20–50 nm were obtained. For the sample in Figs. 3 and 4 it has been found that $\sigma \cong 30$ nm.

One can compute now the spectral dependence of a_r by removing the BA spectral plot from the spectral characteristic of $\ln([1-R^0_{12})(1-R^0_{23}]/T]$. The results after the correction are shown in Fig. 5 for the sample from Figs. 3, 4. Note small differences between $a_r(\hbar\omega)$ plots for different thicknesses of the wafer. The difference between the extreme plots at $a_r = $ const. does not exceed a few meV; i.e., it is below the total error of energy scale estimated to be approximately equal to 10 meV. That procedure has been applied to the samples with different molar content and the results are discussed elsewhere [15].
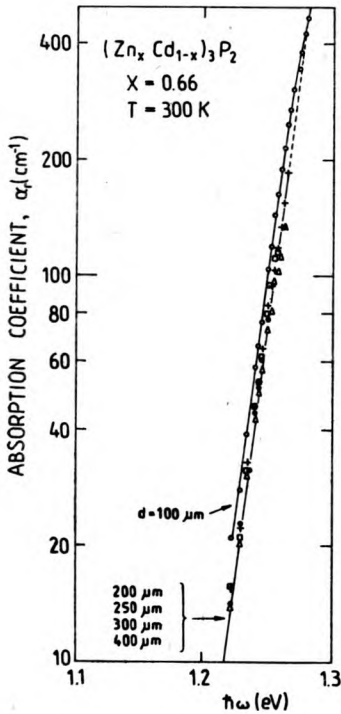
Fig. 5. The absorption coefficient after correction for the BA, a_r, for the sample from Fig. 3. Only exemplary points are shown to clarify the figure

4. Final conclusions

A simple model was proposed to estimate the effect of the surface and volume imperfections upon the results of R and T measurements at normal incidence. Furthermore, the model made it possible (together with the special experimental procedure) to get both terms of the BA (i.e., A_S and a_{im}) separated. It was found experimentally that A_S dominated over the $a_{im}d$ product for samples with $d < 0.2$ mm, approximately, and was of the same order of magnitude as $a_r d$ product (compare Fig. 4 and Fig. 5). Therefore, the estimation of the influence of the surface and volume imperfections (i.e., values of A_S and a_{im}) on the experimental results was crucial to determine the $a_r(\hbar\omega)$ plots as unambigously as possible. Furthermore, the estimation of A_S allowed us to determine the r.m.s. values of the roughness on the samples surfaces, assuming the physical imperfections on the surface to be negligible. It seems to be a reasonable assumption [8]. The values obtained, in the range of 20–50 nm, are reasonably well fitted with the estimation done by surface profile checking. The presented above method of analysis of the absorption coefficient should be applied especially to the samples with rough surface, thin films, etc., in which $A_S > a_{im}d$ and A_S is comparable or even higher than the $a_r d$ product.

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Влияние поверхностных и объемных несовершенств на коэффициент абсорбции образца полупроводника

Обсуждено влияние поверхностных и объемных несовершенств, выступающих в реальном образце полупроводника, на результаты измерения проницаемости и отражения. Обсужден, кроме того, метод расчета коэффициента абсорбции и показан анализ экспериментальных данных, основанный на примерах.