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Ellipsometric investigations of amorphous phase in GaP implanted with Ar^+ ions*

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Ion-implanted GaP was investigated by ellipsometry. The optical constants, the thickness of disordered layer and the degree of amorphousness were determined on the basis of a four-phase model of implanted sample.

1. Introduction

Ion implantation process causes structural changes in the implanted layer. Experimental techniques often used for investigations of damaged layer are electro reflectance [1] or RBS [2], [3]. Ellipsometry is a complementary method for a non-destructive study of implanted semiconductor materials. By means of this method the changes in optical constants, *n* and *k*, induced by ion implantation and a degree of amorphousness can be determined [2]–[11].

2. Experimental

The samples under examinations were (100)-oriented, *n*-type *S* doped GaP crystals having a carrier concentration 5×10^{17} cm^{-3}. GaP samples were implanted 100 keV Ar^+ iones by means of UNIMAS 79 ion accelerator. Before the implantation process the surfaces of all samples were chemically etched in bromo-methanol in order to remove the surface contaminations and to obtain a good optical quality of the surface. Implantation was carried out at 10^{-4} Pa pressure in the sample chamber of accelerator. The density of ion beam current was not greater than 0.1 $\mu A/cm^2$ to

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avoid annealing during implantation. The doses of implanted Ar^+ ions were ranging from 3×10^{12} to 10^{16} cm^{-2}. Ellipsometric measurements for unimplanted and implanted samples were performed with EL11D automatic and EL6 null static ellipsometers. Ellipsometric parameters Ψ and Δ were measured at five wavelengths (450, 500, 550, 600, 632.8 nm) and at angles of incidence from 65 to 72 deg.

3. Theory

For the majority of applications of the reflection ellipsometry, the model of an ideal optically isotropic three-phase system is adequate.

For the case of three-phase system (ambient-film-substrate) the general ellipsometric equation which relates the measured ellipsometric angles Ψ and Δ to the optical properties of the studied system can be written in the form

$$\tan\Psi e^{i\Delta} = \frac{\tilde{r}_{01p}+\tilde{r}_{12p}e^{-i2\beta}}{1+\tilde{r}_{01p}\tilde{r}_{12p}e^{-i2\beta}}\frac{1+\tilde{r}_{01s}\tilde{r}_{12s}e^{-i2\beta}}{\tilde{r}_{01s}+\tilde{r}_{12s}e^{-i2\beta}} \tag{1}$$

where $\tilde{r}_{01p}$, $\tilde{r}_{01s}$, $\tilde{r}_{12p}$, $\tilde{r}_{12s}$ are the ambient-film (01) and the film-substrate (12) interface Fresnel reflection coefficients for the p and s polarization, β is the film phase thickness given by

$$\beta = 2\pi\frac{d_1}{\lambda}(\tilde{n}_1^2-\tilde{n}_0^2\sin^2\varphi_0). \tag{2}$$

In the most cases of practical interest, the medium of incidence (the ambient) has a known refractive index $\tilde{n}_0$ and only the optical parameters of the film substrate subsystem are to be determined. These optical parameters are the complex refractive indices of the film $\tilde{n}_1 = n_F-ik_F$ and the substrate $\tilde{n}_2 = n_s-ik_s$ and the film thickness d_1 for given values of the wavelength λ of the ellipsometer light beam and its angle of incidence φ_0 in the ambient. The functional dependence of Ψ and Δ on the system parameters can be symbolically written as

$$\tan\Psi e^{i\Delta} = \varrho(\tilde{n}_0, \tilde{n}_1, \tilde{n}_2, d_1, \varphi_0, \lambda). \tag{3}$$

Equation (3) may be broken into two real equations for Ψ and Δ, separately:

$$\Psi = \tan^{-1}|\varrho(\tilde{n}_0, \tilde{n}_1, \tilde{n}_2, d_1, \varphi_0, \lambda)|, \tag{4}$$

$$\Delta = \arg[\varrho(\tilde{n}_0, \tilde{n}_1, \tilde{n}_2, d_1, \varphi_0, \lambda)] \tag{5}$$

where $|\varrho|$ and $\arg[\varrho]$ are the absolute value and argument of the complex function ϱ, respectively.

It is being assumed that the ambient, film and substrate media are all homogeneous and optically isotropic and that the refractive index experiences a discontinuous, step-like jumps across the ambient-film and film-substrate parallel plane interfaces. Let multiple-angle-of-incidence measurements be made at M different angles of incidence φ_i [12].

From Equations (1), (4) and (5) $2M$ simultaneous non-linear eqnations are obtained that relate the measured ellipsometric angels Ψ_i^m, Δ_i^m at a given wavelength to the optical parameters n_s, k_s, n_F, k_F and d of the film-substrate subsystem as follows:

$$\Psi_i^m = \Psi_i^c(n_s, k_s, n_F, k_F, d, \varphi_i), \quad (6)$$

$$\Delta_i^m = \Delta_i^c(n_s, k_s, n_F, k_F, d, \varphi_i), \quad (7)$$

(where $i = 1, 2, \ldots, M$), and the superscripts m and c distinguish the measured and computed values of Ψ and Δ, respectively. Because of experimental and/or model errors Eqs. (6) and (7) cannot all be satisfied exactly so that a least-squares solution must be sought.

If the parameters n_s, k_s, n_F, k_F and d are represented as the components of a vector $\boldsymbol{B} = (b_1, b_2, \ldots)$ the computational part of the problem is to find a vector $\boldsymbol{B}_0$ such that the error function

$$G(\boldsymbol{B}) = \sum_{i=1}^{M} \{[\Delta_i^c - \Delta_i^c(\boldsymbol{B}, \varphi_i)]^2 + [\Psi_i^m - \Psi_i^c(\boldsymbol{B}, \varphi_i)]^2\} \quad (8)$$

is minimum. In order to obtain the coordinates of $\boldsymbol{B}$ vector, the minimum of error function was searched with the standard minimization computer programme MINUIT.

4. Results and discussion

The optical constants of unimplanted and implanted GaP samples were determined by using the Multiple Angles of Incidence Ellipsometry MAIE [12].

In the first stage of our calculations, the optical constants n_c and k_c of unimplanted GaP samples were obtained. Ψ^c and Δ^c values were computed with the assumption of a three-phase model of uniplanted crystals (the ambient, the native oxide, the substrate), see Fig. 1. In these calculations it was assumed that the native

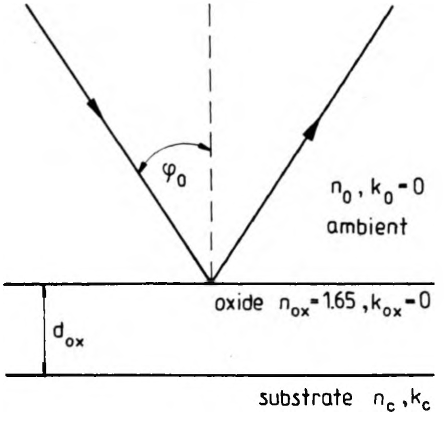

Fig. 1. Three-phase model of unimplanted GaP

oxide formed a plano-parallel and homogeneous layer with an extinction coefficient $k_{ox} = 0$ and a refractive index n_{ox} independent on the wavelength of incident light. On the basis of these assumptions to MAIE method the optical constants n_c and k_c of unimplanted GaP crystals, the refractive index and thickness of the native oxide were calculated (for $\lambda = 632.8$ nm $n_c = 3.305$, $k_c = 0.015$, $d_{ox} = 2.5$ nm). The error function for obtained results was not greater than 0.04.

Optical constants of implanted samples and the thickness of implanted layer were calculated with the same procedure. For these calculations, the four-phase model consisting of the ambient, the native oxide, the implanted layer and the crystalline substrate was employed (Fig. 2). It was assumed that the native oxide layer on the surface of implanted samples has a thickness and a refractive index the same as the oxide on unimplanted samples. The fact that the thickness of disordered layer depends only on the energy of implanted ions and is independent of the dose is very helpful in our numerical calculations [13]. On the basis of the four-phase model and the ellipsometric measurements and of the samples implanted with Ar^+ ions doses ranging from 3×10^{12} to 10^{16} cm^{-2} the minimum of error function $G(\boldsymbol{B}_0)$ was found. The coordinates of $\boldsymbol{B}_0$ vector are the effective refractive index the effective extinction coefficient and the thickness of implanted layer. The optical constants n_{eff} and k_{eff} as a function of the dose are presented in Fig. 3. The thickness of disordered layer calculated from MAIE method is equal to 98 nm. The implanted layer is assumed to be a random mixture of x volume fraction of amorphous phase and $(1-x)$ volume fraction of crystalline phase. The dielectric function of the mixture can be described

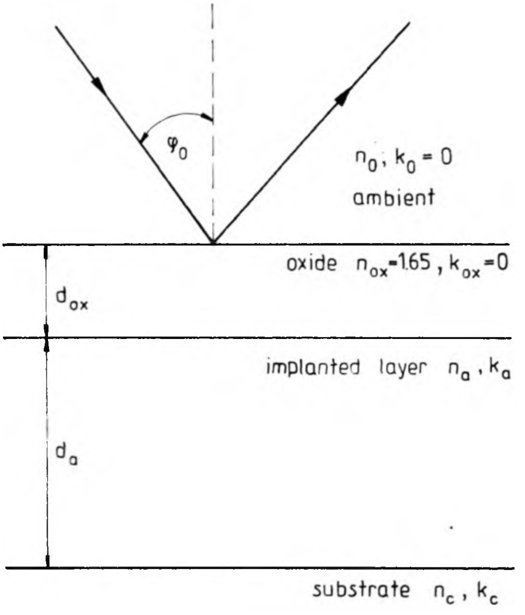

Fig. 2. Four-phase model of implanted GaP

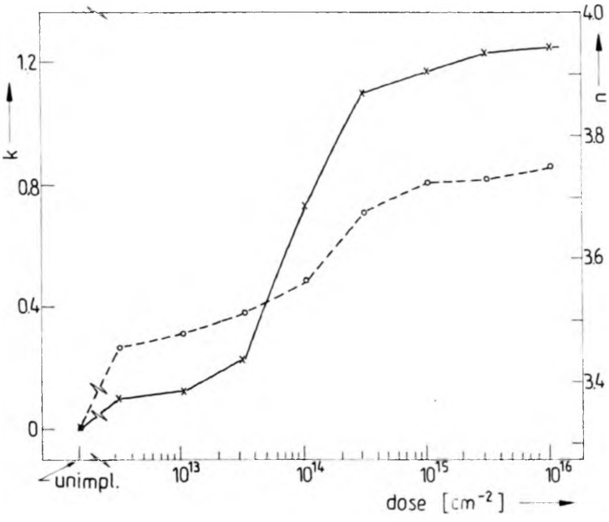

Fig. 3. Optical constants n (solid line) and k (dashed line) of GaP samples implanted with 100 keV Ar^+ ions as a function of a dose ($\lambda = 632.8$ nm)

using the effective medium approximation (EMA) [14], [15]

$$x(\varepsilon_a - \langle\varepsilon\rangle)(\varepsilon_a + 2\langle\varepsilon\rangle)^{-1} + (1-x)(\varepsilon_c - \langle\varepsilon\rangle)(\varepsilon_c + 2\langle\varepsilon\rangle)^{-1} = 0 \tag{9}$$

where: ε — dielectric function of the mixture, ε_c — dielectric function of crystalline substrate, ε_a — dielectric function of amorphous phase. The optical constants of amorphous phase were also computed on the basis of a three-phase model (the ambient, the native oxide, the amorphous phase) of the sample implanted 100 keV Ar^+ ions with the dose 10^{16} cm^{-2}. At this dose the thickness of disordered layer is greater than the light penetration depth in the studied spectral range and the implanted layer is assumed to be totally amorphous. The degree of amorphousness was obtained from the linear regression analysis [6].

5. Conclusions

The optical constants dependence on the dose of implanted ions have shown the rapid increase of n and k at 10^{14} ions/cm^2, see Fig. 3. It can be explained by the connection of the point defects into clusters and then the studied layer becomes totally amorphous. Similar conclusions were drawn in the papers [10], [11].

Figure 4 shows the degree of amorphousness as a function of dose. Similar results were obtained by Götz [16] from the RBS measurements for GaAs. The thickness d_a of disordered layer was compared with the projected range of ions R_p in the LSS profile (Fig. 5). This comparison has shown that the thickness d_a is of the order of $R_p + \Delta R_p$ (for Ar^+ implanted to GaP $R_p = 76.2$ nm, $\Delta R_p = 36.1$ nm [17], [18]). The

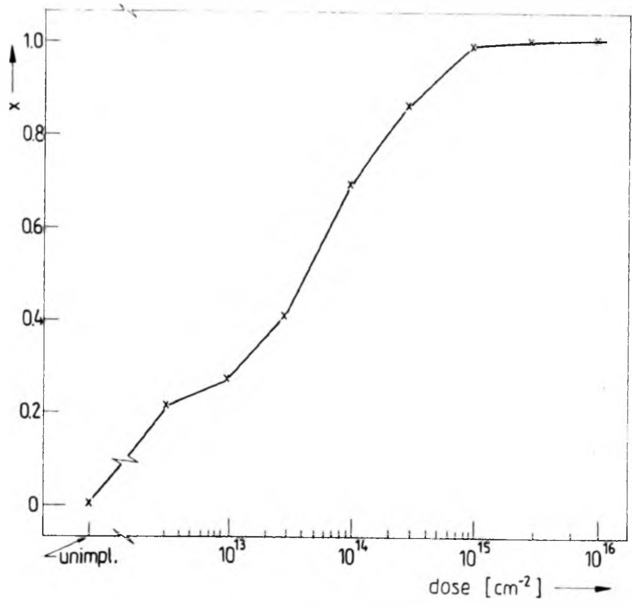

Fig. 4. Degree of amorphousness vs a dose of 100 keV Ar^+ ions implanted to GaP

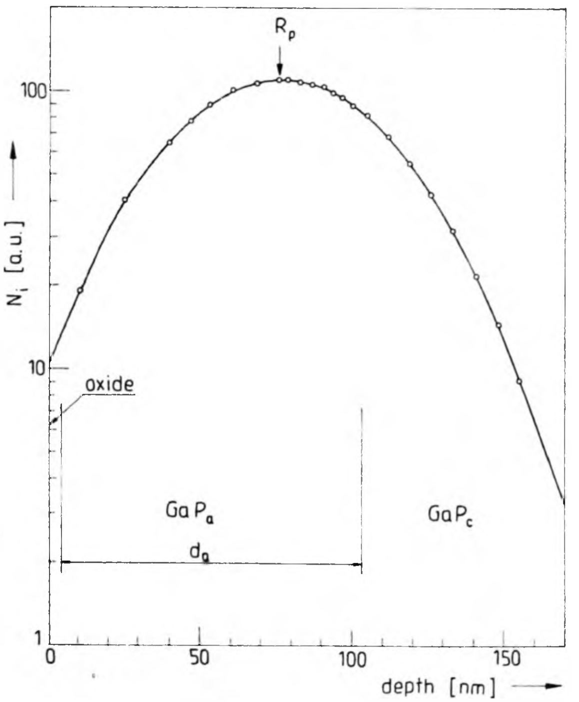

Fig. 5. Thickness of disordered layer d_a in comparison with distribution of implanted ions (Ar^+ 10^{16} cm^{-2}, 100 keV) vs the depth

results obtained have proved that ellipsometry can be a good experimental technique for non-destructive determination of the thickness and the degree of amorphousness of disordered layer in samples of semiconductors after ion implantation.

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Эллипсометрические исследования аморфной фазы в GaP, вводимой ионами Ar^+

Эллипсометрически исследовали ионно вводимый GaP. Оптические постоянные, толщина пленки, разрушенной процессом введения, а также степень аморфизации пленки, определялись на основе четырехфазной модели вводимого материала.