

# **Kramers-Kronig analysis of the optical constants of $Zn_3As_2$ and $Zn_3P_2$ \***

## **IV. Analysis of the accuracy of the applied method of calculation**

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The present paper consists of five parts and is devoted mainly to the results of examination of optical constants in  $Zn_3As_2$  and  $Zn_3P_2$  which are compounds of  $II_3-V_2$  type with broad energy gap. The analysis of the up to now state-of-affairs, so far as the application of the Kramers-Kronig analysis method (KK) for the complex coefficient of reflection is concerned, indicates that it is necessary to develop the research in three additional directions described in the first parts of this series. In the part I a critical analysis of the calculation methods used till now and based on dispersion relations due to Kramers and Kronig has been presented. Also the methods of calculation of optical constants not employing the KK integral have been discussed. In the parts II and III some suggestions of effective improvements of calculation method basing on the KK integrals have been described. Additionally, in both the parts the results of calculations were described for GaAs (as a well known semiconductor) which was employed to test the methods improved by us.

The extensive analysis of errors and accuracies of the calculation methods is given in the present (IV) part of this work. New possible sources of errors are considered and their influence on the final result of calculations is estimated. An illustration of the discussion carried out are the results obtained for GaAs and  $Zn_3P_2$ .

The part V contains the results of calculations of optical constants for  $Zn_3As_2$  and  $Zn_3P_2$ , carried out by using the improved methods of calculation and basing on our own measurements of optical properties of these semiconductors.

## **1. Introduction**

By applying the methods of calculations based on the Kramers-Kronig relations (see the previous parts of this work [1-3]), the spectral characteristics of the complex coefficient of dielectric permittivity and the complex refractive index may be obtained. A problem arises whether and to what degree the estimated values for the optical constants are consistent with their real values. For this purpose it is necessary to consider two possible sources of errors and estimate their influences on the final result of calculations. Similarly, as it was the case in the part III of this work [3], the analysis will be illustrated mainly by the results obtained for reflection spectrum of GaAs after [4].

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## 2. Measurement errors

While measuring the reflection coefficient for a given sample and for given frequency of radiation some spread of results is observed which depends mainly on the quality of the measuring setup. The accuracy of the reflection coefficient measurements in the visible range oscillates between 0.03% [5] and 2% [6]. However, practically much greater spread of results is observed when measuring  $R$  at the given frequency but for different samples. This spread is caused by different surface qualities of particular samples. As it has been shown in paper [7] the differences between the reflection coefficient values for differently prepared surfaces of silicon samples may reach even 30%. Similar results for InAs and InSb have been obtained in paper [8].

Thus, the experimental error of the reflection coefficient may be interpreted as a measure of the spread of results obtained for well prepared sample surfaces or surfaces giving the greatest possible coefficients of reflection for the given material, which are simultaneously characterized by a distinct structure of the reflection spectrum. This error has been estimated, for instance, in the papers [9, 10] to be 5% (measurements for Si and Ge in the 1–10 eV range), in the papers [11] to be 3% (measurements for MoTe<sub>2</sub> in the range 77–6.2 eV), and in the paper [12] to be 1% (measurements for InSe in the range 1.5–5.5 eV).

The measurement error becomes next the source of error  $\Delta\Theta_2^{\text{meas}}$  (an absolute error in the phase change during reflection calculated from the Kramers-Kronig integral in the measurement range (formula (2b) in [3]). Evidently, the error of numerical integration  $\Delta\Theta_2^{\text{calc}}$  should be also taken into account, but it may be assumed that  $\Delta\Theta_2^{\text{calc}} \ll \Delta\Theta_2^{\text{meas}}$ , as it will be shown in the Section 3 of this paper.

By taking advantage of the well known formulae for the real ( $\varepsilon_1$ ) and imaginary ( $\varepsilon_2$ ) parts of the complex coefficient of dielectric permittivity the following relations may be obtained:

$$\Delta\varepsilon_1 = \frac{\Delta R}{R} |(n^2 + x)k| + \Delta\Theta |2n(x - k^2)|, \quad (1a)$$

$$\Delta\varepsilon_2 = \frac{\Delta R}{R} |(x - k^2)n| + \Delta\Theta |2k(x + n^2)|, \quad (1b)$$

where

$$x = [-4R + 2\sqrt{R(1+R)}\cos\Theta][1 + R - 2\sqrt{R}\cos\Theta]^{-2}.$$

When considering the influence of the measurement error,  $\Delta R$ , on the results it is usually assumed that  $\Delta\Theta = \Delta\Theta_2^{\text{meas}}$ . In order to determine  $\Delta\Theta_2^{\text{meas}}$  the calculations were performed for reflection spectra distorted in the error limits so that the discrepancies in the obtained values of  $\Theta_2$  be maximal. The values of  $\Delta\varepsilon_2$  (formula (1b)), obtained for calculations basing on the reflection spectra for GaAs under assumption that  $\Delta R$  amounts successively to 1%, 0.5% and 0.1%, are shown in Fig. 1. Also the spectra of  $\Delta\varepsilon_2/\varepsilon_2$  and  $\varepsilon_2$  are there presented. When examining the effect of the measurement error on the accuracy of the calculated optical constants, the method of calculation, as such, plays a minor role.

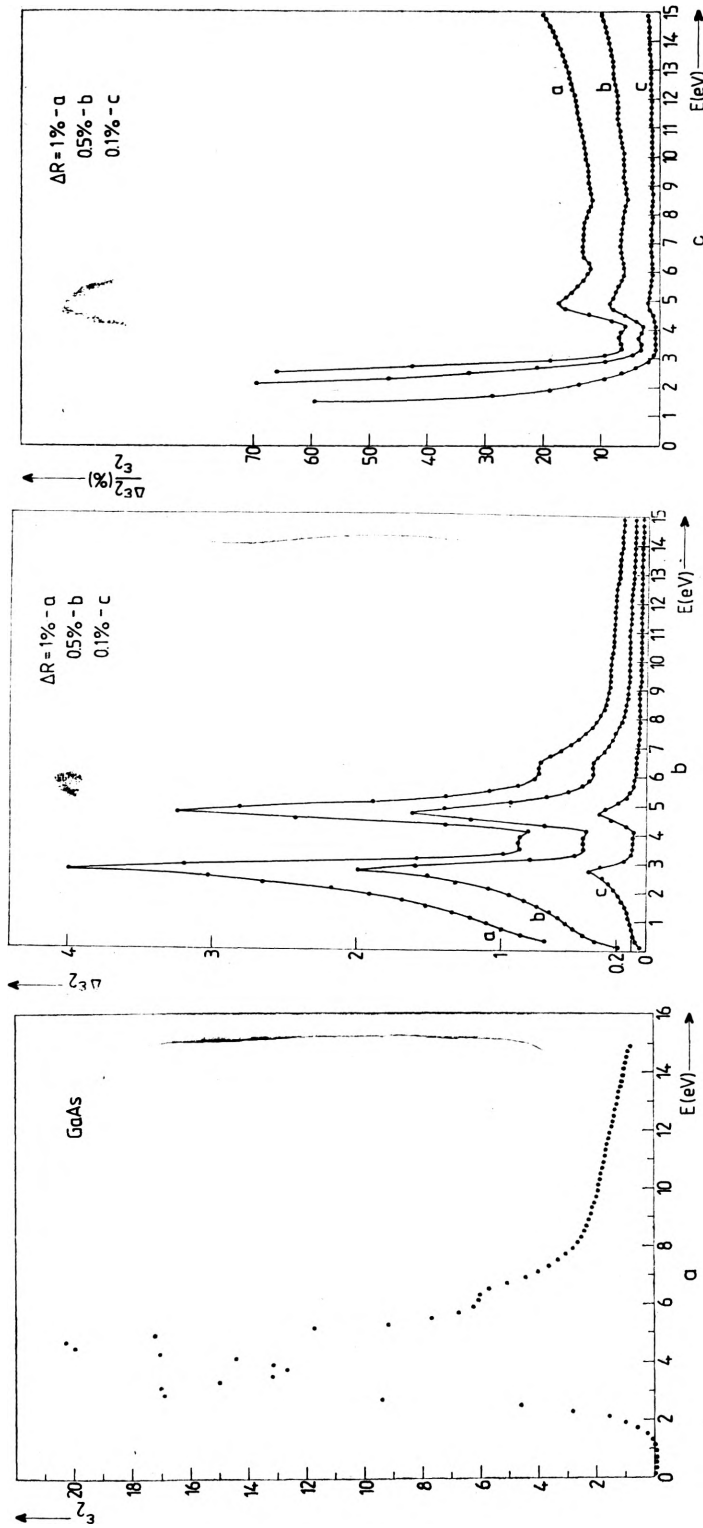


Fig. 1. Imaginary part of the complex coefficient of dielectric permittivity  $\epsilon_2(E)$  (a), calculated for reflection spectrum of GaAs given in the interval 0–1.7 eV by using the Roessler method and both the absolute error  $\Delta \epsilon_2(E)$  (b) and relative error  $\Delta \epsilon_2(E) / \epsilon_2(E)$  (c) caused by the measurement error  $\Delta R$  assumed to be equal to 1%, 0.5% and 0.1%

Hence, in the programme of calculation one of the most simple methods, i.e., Roessler method [1], was used.

When analysing the results obtained, an approximately linear dependence of  $\Delta\varepsilon_2$  and  $\Delta\varepsilon_2/\varepsilon_2$  on the measurement error may be noticed. Also the errors for other optical constants behave similarly. The value  $\Delta\varepsilon_2/\varepsilon_2$  may be estimated to be 10%, 5% and 1% for  $\Delta R$  amounting to 1%, 0.5% and 0.1%, respectively. The regions, in which  $\varepsilon_2$  is close to zero and  $\Delta\varepsilon_2/\varepsilon_2$  reaches very high values, are neglected. It is worth noticing that  $\Delta\varepsilon_2/\varepsilon_2$  has a distinctly visible minimum (of relatively small values) between two principal maxima depending on  $\varepsilon_2(E)$ .

The results show that both the components in eqs. (1a) and (1b) are of the same order within the whole measurement range. This means that the immediate influence of the measurement error  $\Delta R$  as well as its indirect influence through  $\Delta\theta_2^{\text{meas}}$ , thus through  $\Delta\theta$ , on the final value of the calculation error are comparable.

From the comparison of the relative errors of the determined optical constants presented in Fig. 2, it follows that the particular optical constants "react" in different way to the measurement error. The complex coefficient of dielectric permittivity is, in general, determined less accurately than the complex refractive index.

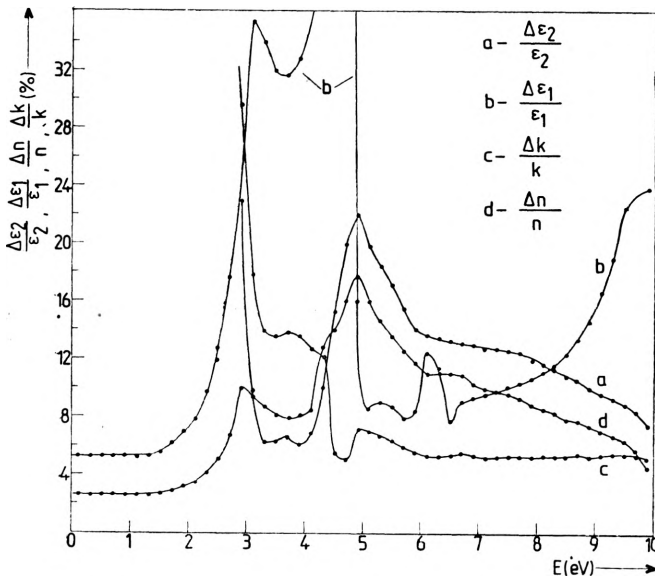


Fig. 2. Relative errors of optical constants of GaAs  $\Delta\varepsilon_1(E)/\varepsilon_1(E)$ ,  $\Delta\varepsilon_2(E)/\varepsilon_2(E)$ ,  $\Delta n(E)/n(E)$ ,  $\Delta k(E)/k(E)$  obtained under assumption that the absolute error of reflection coefficient measurement amounts to 1%. The optical constants have been calculated with the help of Roessler method from the reflection spectrum for GaAs given in the interval 0–10 eV

The further analysis of measurement errors of the optical constant determination indicates a slow increase of these errors with the broadening of the measurement interval.

### 3. Calculation errors

At the beginning a method of determining  $\theta_2$ , i.e., a method of numerical calculation of the integral presented by the formula (2b) in the part III of this work [3], will be given. The measurement interval  $(E_a, E_b)$  is written down as a sum of intervals of the form  $(E_i - \Delta,$

$E_i + \Delta$ ), where  $E_i$  changes from  $E_a + \Delta$  to  $E_a - \Delta$ , each  $2\Delta$ . Hence

$$\Theta_2(E) = \frac{E}{\pi} P \int_{E_a}^{E_b} \frac{\ln R(x)}{E^2 - x^2} dx = \frac{E}{\pi} \sum_i P \int_{E_i - \Delta}^{E_i + \Delta} \frac{\ln R(x)}{E^2 - x^2} dx. \quad (2)$$

Next, the function  $\ln R(E)$  obtained from measurements is approximated in the segment  $(E_i - \Delta, E_i + \Delta)$  by a straight line, which reduces the problem to solving the system of equations:

$$\begin{aligned} (E_i - \Delta) a_i + b_i &= \ln R(E_i - \Delta), \\ (E_i + \Delta) a_i + b_i &= \ln R(E_i + \Delta). \end{aligned} \quad (3)$$

The formula (2) takes the form

$$\Theta_2(E) = \frac{1}{2\pi} \sum_i \left\{ a_i E \ln \left| \frac{(E_i - \Delta)^2 - E^2}{(E_i + \Delta)^2 - E^2} \right| + b_i \ln \left| \frac{(E + \Delta)^2 - E_i^2}{(E - \Delta)^2 - E_i^2} \right| \right\}, \quad (4)$$

where  $E \neq E_i \pm \Delta$  for each  $i$ .

The integrating subroutine has been checked for several simple functions, for which the integral (2) may be calculated analytically. The errors oscillated from  $10^{-4} / 0$  to  $1^0 / 0$ , with the exception of regions where  $\Theta_2$  was close to zero. However, this is by no means a good way of estimating the calculation error for this concrete case.

It should be noticed that the reflection spectrum is given in a discrete way and the run of the  $R(E)$  curve between the measurement points is known. It seems to be reasonable to assume that within those rather narrow regions the  $R(E)$  has no extremes. This results in a simple method of numerical integration, which allows to determine the error  $\Delta\Theta_2^{\text{calc}}$ . A division of the measurement interval  $E_a = E_a < E_2 \dots < E_i < \dots < E_n = E_b$  is made so that  $E_1, E_2, \dots, E_n$  be the measurement points, and it is assumed that  $R(E) = R(E_i)$  or  $R(E) = R(E_{i+1})$  along the segment  $(E_i, E_{i+1})$ . The maximal value of  $\Theta_2$ , i.e.,  $\Theta_2^{\text{max}}$ , and minimal value of  $\Theta_2$ , i.e.,  $\Theta_2^{\text{min}}$  may be now calculated from the following relations

$$\begin{aligned} \Theta_2^{\text{max}}(E) &= \frac{1}{2\pi} \sum_{i=1}^{n-1} \{ \max [\ln R(E_i) A_i, \ln R(E_{i+1}) A_i] \}, \\ \Theta_2^{\text{min}}(E) &= \frac{1}{2\pi} \sum_{i=1}^{n-1} \{ \min [\ln R(E_i) A_i, \ln R(E_{i+1}) A_i] \}, \end{aligned} \quad (5)$$

where

$$A_i = \ln \left| \frac{(E + E_{i+1})(E - E_i)}{(E - E_{i+1})(E + E_i)} \right|.$$

Now, it remains to determine  $\Theta_2$  and  $\Delta\Theta_2^{\text{calc}}$

$$\Theta_2 = \frac{1}{2} (\Theta_2^{\text{max}} + \Theta_2^{\text{min}}), \quad (6)$$

$$\Delta\Theta_2^{\text{calc}} = \frac{1}{2} (\Theta_2^{\text{max}} - \Theta_2^{\text{min}}). \quad (7)$$

Clearly, the difference between  $\Theta_2$  calculated according to (4), and  $\Theta_2$  determined from the formula (7) for the same density of the measurement points is less than  $\Delta\Theta_2^{\text{calc}}$ .

As it follows from the results, the absolute error  $\Delta\Theta_2^{\text{calc}}$  (formula (7)) is approximately directly proportional to  $\Delta$ , ( $\Delta = E_{i+1} - E_i$ ), i.e., to the distance between the two successive measurement points.  $\Delta\Theta_2^{\text{calc}}$  exhibits also a small increase when the measurement interval is subject to extension.

The condition  $\Delta\Theta_2^{\text{calc}} \ll \Delta\Theta_2^{\text{meas}}$  requires that for the given  $\Delta R$  the measurements be sufficiently dense. For the values of  $\Delta R$  used in practice the required measurement density may be easily achieved. The fulfilment of the said condition in a concrete case of reflection spectrum of  $\text{Zn}_3\text{P}_2$  (optical constants of  $\text{Zn}_3\text{P}_2$  will be more accurately discussed in the part V of this work [13]) for  $\Delta R = 1\%$  and  $\Delta = 0.04$  eV, is illustrated in Fig. 3.

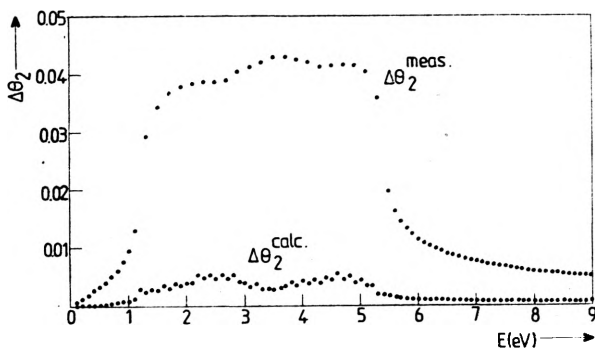


Fig. 3. Relative errors  $\Theta_2$  caused by the measurement error  $\Delta R$  (amounting to 1%)  $\Delta\Theta_2^{\text{meas}}$ , and by the error due to discrete measurement of reflection coefficient in 0.04 eV steps,  $\Delta\Theta_2^{\text{calc}}$ . The calculations have been performed for the reflection spectrum of  $\text{Zn}_3\text{P}_2$  given in the interval 1.20–5.4 eV

The calculation error is connected also with determination of  $\Theta_1$  and  $\Theta_3$ , i.e., with determination of the contributions to  $\Theta$  from the regions of low- and high-energy extrapolation. Here, simple manipulation, like summing the suitably large number of components in the series in the formula (6) [3], suffices to make the calculation error in these cases much less than  $\Delta\Theta_2^{\text{meas}}$ .

#### 4. Extrapolation errors

The extrapolation of the reflection curve outside the final measurement points is also an essential source of errors. Here, the errors due to application of a concrete extrapolation method (which is essentially a set of assumptions and a calculation algorithm for extrapolation parameters) as well as the errors due to nonuniqueness of the extrapolation method may be distinguished.

The latter type includes the error caused by the arbitrariness of selection of some parameters for the given extrapolation method. The said spread of results increases with the increase of energy when the zeroing condition for 0 below the absorption edge is employed. This is so, for instance, in the Philipp-Taft method (see Section 2, in paper [3]), when the exponent  $A$  is chosen arbitrarily from the interval  $(-4, 0)$  and  $E_f$  is determined from the condition of zeroing of  $\Theta$  in the least-square sense within the region of transparency (Fig. 4). The described nonuniqueness may be reduced significantly at the expense

of some complication of the given calculation method. Thus, the variant of the Philipp-Taft method mentioned above should be modified to enable  $A$  to be determined uniquely by taking the maximal value of  $E_f$ . Such a modification of the method is not always possible, since often the additional conditions to be imposed on the extrapolation parameters are difficult to formulate.

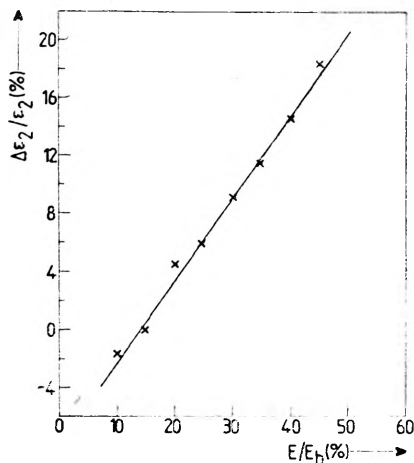


Fig. 4. Estimation of the relative error  $\Delta\epsilon_2/\epsilon_2$  for the Philipp-Taft method following from the arbitrary choice of the parameter  $A$  (see text). Calculations were carried out for the reflection spectrum for GaAs in the interval (0, 25.4) eV

In the analysis of the error due to nonuniqueness of the extrapolation method, the attention should be also paid to the error caused by the fact that the quantities used are already loaded with an error. Here, the zeroing condition for  $\Theta$  (mentioned many times above) in the region of transparency should be recalled in the first place. When knowing  $\Theta_1(E)$  and  $\Theta_2(E)$  the extrapolation parameters are determined so that  $\Theta_3(E) = -\Theta_1(E) - \Theta_2(E)$  for  $E < E_g$ . The fact that  $\Theta_3$  is less sensitive to the values of extrapolation parameters in the transparency region (the latter being usually positioned at a significant distance from the extrapolation region) than in higher energies, is very disadvantageous. Thus, even small calculation errors for  $\Theta_1$  and  $\Theta_2$  may cause such changes in the determined parameters that essential divergences in the determined optical constants may occur for higher energies.

The error discussed above may be reduced by increasing the accuracy of measurement or by slight modification of the calculation method.

The error caused by the choice of a concrete extrapolation method creates much greater problem. Here the difficulty is due to the fact that the behaviour of the reflection spectrum outside the end measurement point is known only in very general terms. It is well known that in this region the reflection coefficient is small and that some structures connected with high energy transitions may appear. Besides, the reflection coefficient must diminish like  $E^{-4}$  for high energies, as it follows from the general principles. This assumption admits a very great variety of possible extrapolations. It seems also that the extrapolation consistent with reality will differ significantly from the simple models of the type  $R(E) = BE^A$ . Hence, the chosen extrapolation reflects not so much the real behaviour of  $R(E)$  for high energy but it rather enables the fulfilment of the basic condition, i.e., that of zeroing of  $\Theta$  in the transparency region. It may be easily imagined that many ex-

trapolations may fulfil this condition in a satisfactory way. The degree to which the estimated optical constants depend upon the concrete form of extrapolation will increase with the increasing energy. In order to estimate the error of the extrapolation method produced in this way, the knowledge of all the correct extrapolations, i.e., the extrapolations fulfilling satisfactorily the basic conditions given above, seems to be necessary.

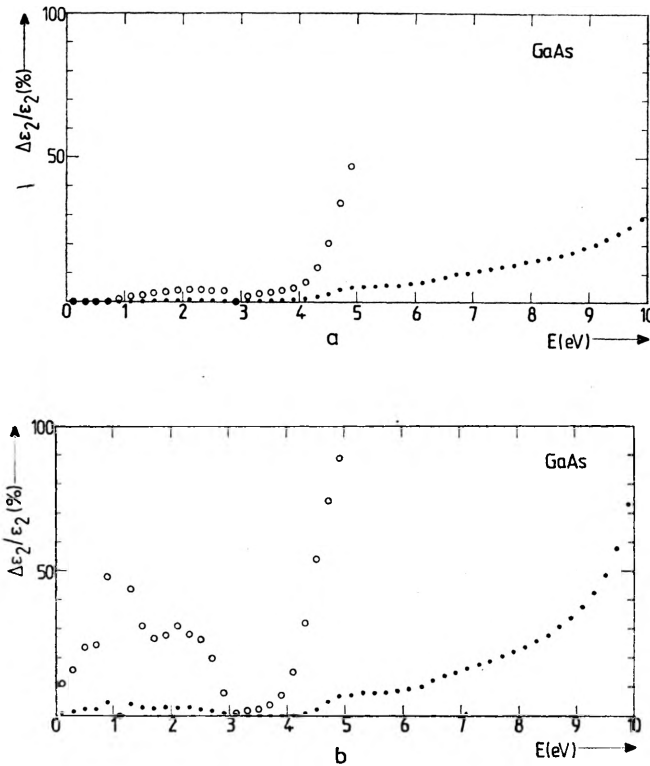


Fig. 5. Relative change in the imaginary part of the complex dielectric permittivity  $\Delta\epsilon_2/\epsilon_2$  caused by reduction of the measurement range to 10 eV (...) and to 5 eV (oooo) for the SKK method (a) and that of Roessler (b). The test has been carried out for the reflection spectrum of GaAs given in the interval (0, 25.4) eV

One of the estimation methods used for extrapolations consists in gradual reduction of the measurement range for the benefit of the extrapolation region. In this case, the smaller are the divergences of the optical constants the better the calculation method used [14]. Such tests have been carried out for the Roessler method (Section 3.1, part I [1]), and the SKK method (Section 2, part II, [2]). The spectrum of reflection for GaAs in the region 0–25.4 eV [4] has been taken for calculations. Next, the upper bound of this range was reduced to 10 eV and to 5 eV, respectively. The relative change of  $\epsilon_2$  during this procedure is presented in Fig. 5. It may be seen that the SKK method is less sensitive to the reduction of the measurement region than the Roessler method. It seems that this may be a premise to the statement that the error is smaller for the SKK method.

In order to verify the results of optical constants and also to estimate the method of calculation (to some extent) the rules of summation may be used, which will be discussed in the next Section.



## 5. Summation rules

For the spectral dependences of optical constants as well as for the functions of these constants a number of relations may be written in which the knowledge of the optical constants for high energy region is exploited. These dependences are based on the dispersion relations and bear the common name of summation rules. The exemplified derivation (according to the [15]) of one of the most known summation rules is given in the Appendix.

The high versatility of the summation rules may be illustrated by the following list. In the formulae the notations used commonly for complex reflection coefficient  $\hat{r} = \sqrt{R}e^{i\theta}$ , complex refractive index  $\hat{n} = n + ik$ , complex dielectric permittivity  $\hat{\epsilon} = \epsilon_1 + i\epsilon_2$  and also plasma energy  $E_p$  have been employed. The relations will be given in the form valid for uniform and isotropic semiconductor:

$$\int_0^{\infty} x\epsilon_2(x) dx = \frac{\pi}{2} E_p^2, \quad (8)$$

$$\int_0^{\infty} xk(x) dx = \frac{\pi}{4} E_p^2, \quad (9)$$

$$\int_0^{\infty} [n(x) - 1] dx = 0, \quad (10)$$

$$\int_0^{\infty} [\epsilon_1(x) - 1] dx = 0, \quad (11)$$

$$\int_0^{\infty} xk(x) [n(x) - 1] dx = 0, \quad (12)$$

$$\int_{-\infty}^{+\infty} x^{2m-1} [\hat{n}(x) - 1]^m dx = (-1)^m 2^{-m} i \pi E_p^{2m}, \quad m \geq 1, \quad (13)$$

$$\int_{-\infty}^{+\infty} x^{2m-1} [\epsilon(x) - 1]^m dx = (-1)^m i \pi E_p^{2m}, \quad m \geq 1, \quad (14)$$

$$\int_0^{\infty} [n^2(x) - k^2(x) - 2n(x) + 1] dx = 0, \quad (15)$$

$$\int_0^{\infty} [n(x) - 1] \{ [n(x) - 1]^2 - 3k^2(x) \} dx = 0, \quad (16)$$

$$\int_0^{\infty} xR(x) \sin 2\theta(x) dx = 0, \quad (17)$$

$$\int_0^{\infty} R(x) \cos 2\theta(x) dx = 0. \quad (18)$$

The derivation and discussion of the above formulae may be found in literature and in particular: the formulae (9) and (10) in [16], the formula (1) in [17], the formulae (12)–(14) in [18] the formulae (15) and (16) in [19] and (17) and (18) in [20].

After having calculated the optical constants from the dispersion relations the summation rules may be used to verify the results obtained. The rules (8)–(11) are especially important, since they enable to test each optical function separately, moreover, there are no parameters in the eqs. (10) and (11) the knowledge of which would be necessary. Such integrals like (13) and (14) or (8) and (9) are employed, but more frequently to determine the plasma energy than to test the results of calculation and, speaking more strictly, to find the effective number of electrons included in  $E_p$  as a function of the upper limit of integration (see also the Section 5, part II [2]). The relations (15) and (16) are very convenient in applications, since the integrand diminishes quicker (like  $x^{-2}$  and  $x^{-4}$  successively) than in other relations. Thus, it may be expected that the eqs. (15) and (16) will be satisfied with high accuracy even for not too wide integration intervals, provided that the proper calculation method is applied.

Unfortunately, there exist no summation rules that might be used to direct verification of the extrapolation of the refractive coefficient. The reason for this is the fact that  $\ln R(E) = 0(\ln E)$ , when  $E \rightarrow \infty$ . However, the rules of summation for refraction coefficient and the phase changes during the reflection described by the formulae (17) and (18) may be derived in a simple way, but these relations seem to be of small effectiveness in practice.

Very rarely the summation rules play a dominant part in the calculation methods of optical constants. An interesting exception is the method suggested in 1975 by ELLIS and STEVENSON in [21]. This is a variant of the Philipp-Taft method, in which the parameter of extrapolation (exactly the exponent  $A$  from the relation  $R(E) = R(E_b)(E/E_b)^A$ ) is chosen so, that the summation rule given by (12) are fulfilled with the following accuracy

$$\left| \int_0^{140 \text{ eV}} x k(x)[n(x)-1] dx \right| < 0.01. \quad (19)$$

Thus, the summation rules may be very helpful in determining the optical constants with the help of dispersion relations.

## 6. Conclusions

The final results of measurements and the calculations are loaded with the errors coming from many sources. The considerations concerning the measurement, calculation and extrapolation errors lead to important conclusions. It turns out that the least contribution to the global error is due to calculation error. When neglecting this error a coarse analysis of errors may be made but it should be remembered that this is not allowed when a more accurate analysis is needed or when relatively accurate measurements are available.

The main role is played by measurement and extrapolation errors. They differ essentially due to the fact that the influence of the measurement errors on the final results may

be determined very precisely, while in principal, the same cannot be made with the extrapolation error. In estimation of this error there appears a difficulty caused by the fact that the magnitude of the difference between the assumed extrapolation curve and real reflection coefficient in the extrapolation regions is unknown. On the other hand, this difference affects the determination of optical constants and this influence increases with energy. Hence, the search of a method enabling an accurate estimation of the error of the extrapolation method seems to be justified.

Thus, the error of optical constants is in practice defined mainly by the error of the reflection coefficient measurements. The fact that the error of optical constants reaches high values justifies the attempts to determine the measurement error in a most precise way. The dependence of the measurement error upon the energy should be taken into account and also this error should be minimized in a reasonable way.

Finally, there remains a large group of errors connected with the fact that the measurement results are processed basing on a very simple physical model. This group includes the errors caused by the formulae valid for normal light incidence on the sample (while in reality the incidence angle amount to 5–10 degrees of arc) as well as the errors caused by the deviations of the real semiconductor crystal from uniformity and isotropy. It is assumed that all these errors are much less than the errors mentioned above.

## Appendix

The main assumption accepted to derive the summation rules for optical constants is that the response of the medium to the electromagnetic field of high frequencies is similar to the reaction of the free electron gas, i.e., that the Drude formula is valid

$$\epsilon_1(E) \xrightarrow{E \rightarrow \infty} 1 - \frac{E_p^2}{E^2}, \quad (\text{A.1})$$

where  $E_p^2 = (\hbar\omega_p)^2 = \frac{4\pi\hbar^2 N e^2}{m_0}$ ,  $N$  – electron concentration in crystal,  $m_0$  – mass of free electron.

The dispersion relation between  $\epsilon_1$  and  $\epsilon_2$  has the form

$$\epsilon_1(E) - 1 = \frac{2}{\pi} P \int_0^{\infty} \frac{x \epsilon_2(x)}{x^2 - E^2} dx. \quad (\text{A.2})$$

Let  $E_c$  be the cut-off energy, above which there is no absorption. Then  $\epsilon_2(E) = 0$  for  $E > E_c$ . If  $\epsilon_1(E)$  is determined for  $E \gg E_c$ , then  $x$  in the denominator of the first integral in the expression

$$\epsilon_1(E) - 1 = \frac{2}{\pi} P \int_0^{E_c} \frac{x \epsilon_2(x)}{x^2 - E^2} dx + \frac{2}{\pi} P \int_{E_c}^{\infty} \frac{x \epsilon_2(x)}{x^2 - E^2} dx. \quad (\text{A.3})$$

may be neglected. The second integral disappears, since  $\epsilon_2(E) = 0$  for  $E > E_c$ . Hence,

$$\epsilon_1(E) = 1 - \frac{2}{\pi E^2} \int_0^{E_c} x \epsilon_2(x) dx, \quad E \gg E_c \quad (\text{A.4})$$

By taking account of the formulae (A.1) and (A.2) the known summation rule may be obtained for  $\varepsilon_2(E)$

$$\int_0^{\infty} x\varepsilon_2(x)dx = \frac{\pi}{2} E_p^2, \quad (\text{A.5})$$

where the upper integration limit is extended to infinity since  $\varepsilon_2(E)$  disappears for  $E > E_c$ .

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## Определение оптических констант полупроводников $Zn_3As_2$ и $Zn_3P_2$ с помощью соотношения Крамерса-Кронига

### Часть IV. Анализ точности применяемых методов расчёта

Настоящая работа состоит из пяти частей и посвящена главным образом результатам исследований оптических констант  $Zn_3As_2$  и  $Zn_3P_2$  двух соединений типа  $III-V_2$  с широким энергетическим интервалом. Результатом анализа существующего до настоящего времени состояния в области применения метода анализа Крамерса-Кронига (КК) для комплексного коэффициента отражения оказалась необходимость развития работ в дополнительных направлениях, описанных в трёх первых частях. В I части представлен критический анализ применяемых до настоящего времени методов расчёта, основанных на дисперсионных соединениях Крамерса-Кронига. Обсуждены также методы расчёта оптических констант, в которых не используется интеграл КК. Во II и III частях описаны предложения эффективных усовершенствований методов расчёта, основанных на применении интеграла КК. Дополнительно в обеих частях представлены результаты расчёта для

GaAs, который послужил (в качестве полупроводника со сравнительно хорошо известными оптическими свойствами) для проверки усовершенствованных нами методов расчёта.

Анализ ошибок и точности методов расчёта очень подробно проводится в настоящей (IV) части работы. Рассмотрены возможные источники ошибок, а также оценено их влияние на конечный результат расчёта. Иллюстрацией для проведённой дискуссии являются результаты, полученные для GaAs, а также  $Zn_3P_2$ .

Пятая часть содержит результаты расчёта оптических констант  $Zn_3As_2$  и  $Zn_3P_2$ , произведённых с помощью усовершенствованных методов расчёта, а также на основе наших результатов измерений оптических свойств этих полупроводников.