

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

## V. Optical constants of $Zn_3As_2$ and $Zn_3P_2$

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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 three parts of this series. In the part I a critical analysis of the calculation method 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 methods basing on the KK integrals have been described. Additionally, in both the parts the results of calculations were shown for GaAs (as a semiconductor of relatively well known optical properties), which was employed to test the methods improved by us. An extensive analysis of errors and accuracies of these methods has been given in the part IV.

The present (V) part of this work contains the results of calculations for  $Zn_3As_2$  and  $Zn_3P_2$  carried out with the help of improved methods and basing on our own results of measurements. The measurements of the reflection coefficients have been performed at 300 K in nonpolarized light and spectral characteristics of the real and imaginary parts of the complex dielectric constants for both the semiconductors have been calculated and discussed.

## 1. Introduction

The purpose of our work was to determine optical constants of two wide-gap compounds from the  $II-V$  group, i.e., zinc arsenide  $Zn_3As_2$  and zinc phosphide  $Zn_3P_2$ . To this end two tasks seem to be of basic importance: a detailed discussion of the known methods of Kramers-Kronig analysis including suggested modifications of some of them, and the measurements of the reflection coefficients from the surface of  $Zn_3As_2$  and  $Zn_3P_2$  samples, on the base of which the spectral characteristics of optical constants of these compounds have been calculated. The first task was the subject of the previous parts of this work and the results obtained were described there in details [1]. The realization of the second task together with the discussion of the obtained results is presented in the present part of the work.

\* Work sponsored under the Research Project PR-3.08.

## 2. Reflection coefficient from $Zn_3As_2$ and $Zn_3P_2$

### 2.1. Preparation of samples

Monocrystals of  $Zn_3As_2$  and  $Zn_3P_2$  obtained from the gas phase by F. Królicki (Institute of Inorganic Chemistry and Rare Earth Metallurgy, Technical University of Wrocław, Poland) were used to measurements. The details concerning technology of producing both the compounds may be found in paper [2].

In our experiments well-shaped monocrystals of  $d \cong 1$  mm thickness of the above compounds were measured. The crystal structure of  $Zn_3As_2$  sample surface was determined at the Institute of Low Temperature and Structural Research of The Polish Academy of Sciences, Wrocław, Poland. Unfortunately, the surface orientation of the  $Zn_3P_2$  samples failed.

The measurements were carried out both on the samples subject to surface processing (grinding, polishing and etching) and on the mirror surfaces of the crystals processed neither mechanically nor chemically.

### 2.2. Measurements apparatus

The method of measurement of absolute reflection coefficient was employed at almost perpendicular incidence ( $6-7^\circ$ ) of radiation, the scheme of the measurement set-up is presented in Fig. 1, and its detailed description is given in paper [3].

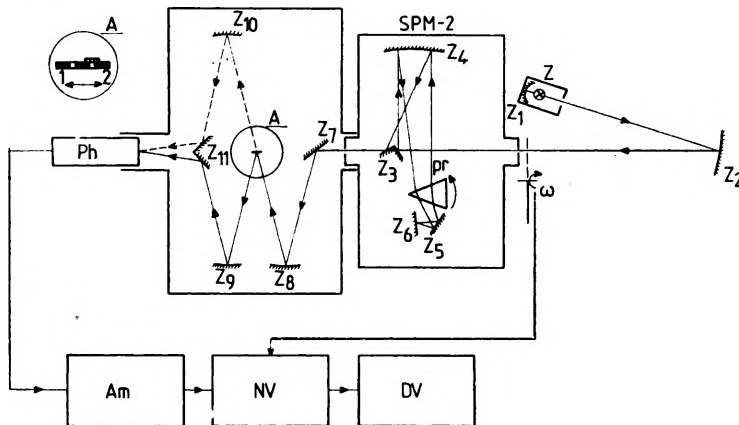


Fig. 1. The measurement setup to measure the reflection in the monochromatic light ( $Z$  — radiation source,  $A$  — holder with the measured sample,  $Ph$  — photomultiplier or other detector,  $Am$ ,  $W$  and  $DV$  are amplifier, nanovoltmeter and a recording arrangement or a digital voltmeter, respectively)

The sample was fixed in a special holder  $A$  which was shifted perpendicularly to the run of the incident ray and could take two positions: in the first position the radiation fell indirectly on the sample (measurement of the intensity of the reflected radiation), in the second one, the radiation passed through the hole, the area of which was equal to the illuminated area of the sample (measurement of the intensity of radiation falling on the sample).

### 2.3. Method of measurement

The measurements were carried out "point after point", five times for each energy of the incident photons. The average value taken of these five measurements was treated as the value  $R$  for the given energy. Such measurements were carried out three times for each sample in the examined interval of energy and a final graph of  $R(E)$  has been made after having averaged the results for respective three measurements.

The measurements were carried out for the monochromator slit within the limits 0.02–0.004 mm which gives the spectral width of the beam of falling photons not greater than 0.004 eV [3]. The error of measurement of the reflection coefficient for single sample was estimated to be 1%. A comparison of results obtained for different samples gives an error in determining  $R(E)$  of order of 5%. Slight changes of the reflection coefficient (of order of 0.5%) as a function of time were also stated during the measurement.

### 2.4. Measurements of the spectral characteristics $(R)E$ for $Zn_3As_2$

The measurements were carried out at the temperature of 300 K on the single crystal samples within the 1.0–5.4 eV range of the photon energies. The samples of surface orientations (001), (010) and (100) have been measured. One of them (sample RA-1) was subject to mechanical and chemical processing described above, while the others remained unprocessed. Typical results are shown in Fig. 2. In spite of the fact that the absolute value

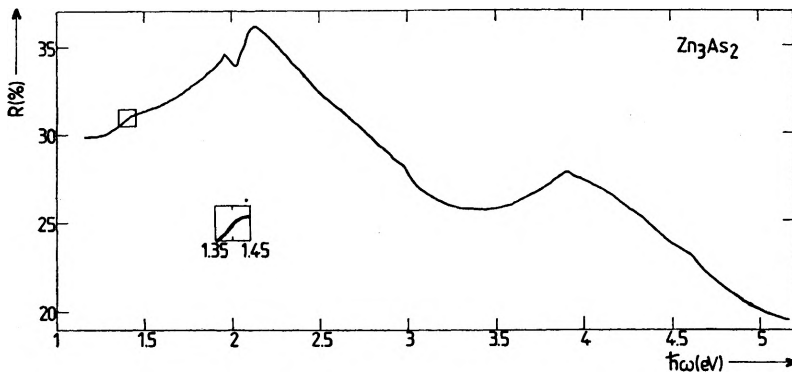


Fig. 2. Exemplified reflection spectrum from the  $Zn_3As_2$  crystal

of the reflection coefficient was proved to depend upon the quality of the prepared surface, the curves  $R(E)$  for different samples pointed out a very high qualitative consistence. They were also consistent with the results of the work [4].

For energies of about 2.10 and 3.90 eV two distinct maxima are observed, the first being higher by about 8.5%. The transitions in the vicinity of  $E = 3.0$  and 4.6 eV and the splitting of the principal maximum were (except for one sample) weakly seen. The characteristic energy of 1.4 eV (unobserved in [4]) was detected in these measurements. This transition was reported in [5], where the thermoreflexion from  $Zn_3As_2$  was measured for the energy of 1.45 eV.

### 2.5. Measurement of the spectral dependence of $R(E)$ for $Zn_3P_2$

The measurements of the nonoriented single crystal samples (of unprocessed surface) have been carried out at the temperature of 300 K within the 1.0–5.4 eV energy range. Two samples were additionally subject to mechanical and chemical treatments. The results are shown in Fig. 3. No essential differences have been stated in the spectrum shape for both natural mirror type samples and those subject to processing. Two observed distinct maxima for energies of about 2.60 and 4.30 eV seem to be of complex structure.

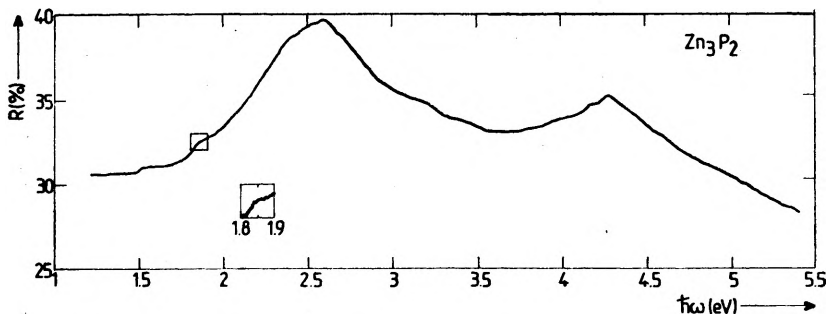


Fig. 3. Exemplified reflection spectrum from the  $Zn_3P_2$  crystal

The majority of observed transitions remain in a good agreement with the results described in [6]. The characteristic energies of about 2.4 and 2.5 eV observed additionally seem to create a subtle structure of two main maxima, while the transition of energy of 1.51 eV is in good agreement with the direct energy gap width determined from the absorption measurement and amounting to 1.505 eV at 300 K [7]. The maxima for 2.63 and 4.32 eV were also observed in the work [8].

### 3. Optical constants of $Zn_3P_2$

$Zn_3P_2$  is a semiconductor compound of  $p$ -type belonging to the compound group  $A^{II}B^V$ . The known physical properties of this compound have been described in paper [9], optical examinations of the band structure of this compound and the values of the energy gap at different temperatures being discussed in details in [10]. Among others, the estimated value of the oblique energy gap of  $Zn_3P_2$  amounts to 1.315 eV, while the direct energy gap is equal to 1.505 eV at 300 K.

In the present work calculations of the optical constants  $Zn_3P_2$  have been carried out by using three methods: (i) Philipp-Taft method in modified version described in the part III of our work [1], (ii) modified SKK method described in the part II of this work [1], and (iii) the method of "power series" described in parts I and III of this work [1].

### 3.1. Calculations by the Philipp-Taft method

The method of calculations was based on extrapolation of  $R(E) = \text{const.}$  up to energy, which had been determined by fulfilling (in the least-square sense) the condition of zeroing  $\Theta$  below the energy  $E_g$ . Here, the formula (see [1], part III)

$$R(E) = R(E_b) \left( \frac{E}{E_b} \right)^A, \quad (1)$$

was used, where  $E_b$  is the end of the measurement range, and

$$A = \left[ \Theta_1(E_0) + \Theta_2(E_0) + \frac{\ln R(E_b)}{2\pi} \ln \frac{(E_b - E_0)(E_f + E_0)}{(E_b + E_0)(E_f - E_0)} \right] \times \left\{ \frac{1}{\pi} \sum_{m=0}^{\infty} \left[ \left( \frac{E_0}{E_b} \right)^{2m+1} - \left( \frac{E_0}{E_f} \right)^{2m+1} \right] \frac{1}{(2m+1)^2} \right\}^{-1}, \quad (2)$$

$E_f$  is the fitting parameters. The formula (1) was applied in the energy range  $(E_b, E_f)$ , while the extrapolation according to formula

$$R(E) = R(E_f) \left( \frac{E}{E_f} \right)^{-4} \quad (3)$$

was additionally performed within the range  $(E_f, \infty)$ . A detailed discussion of the formula is given in part III of the work [1].

The measurements of the reflection coefficient in the range 1.2–5.4 eV made for one of the samples (No. *RP-10*) were exploited in calculations. Since the measurement range was too small to apply successfully this method of calculations, the measurement data were completed within the range 5.4–11.6 eV by the data taken from the work [6]. The value of the fitting parameter was assumed to be  $E_f = 46.03$  eV. The calculated values of optical constants are presented in Fig. 4a.

### 3.2. Calculations by SKK method

In calculations of optical constants made with the help of this method, the quick convergence (of  $1/E^4$  type) of the integral

$$\Theta_{SKK}(E) = E \left[ \frac{1}{\pi} P \int_0^{\infty} \frac{(E_0^2 - E^2) \ln R(E)}{(E_0^2 - x^2)(E^2 - x^2)} dx + \frac{\Theta(E_0)}{E_0} \right] \quad (4)$$

is exploited. When knowing the values of  $R(E)$  in the measurement limits  $(E_a, E_b)$  it is assumed that

$$R(E) = \begin{cases} R(E_a), & E \in (0, E_a), \\ R(E_b), & E \in (E_b, \infty). \end{cases} \quad (5)$$

The integral (4) takes now the analytic forms, given in the part II of paper [1] by the formulae (13)–(15), for the intervals  $(0, E_a)$ ,  $(E_b, \infty)$  and  $(E_a, E_b)$ , respectively.

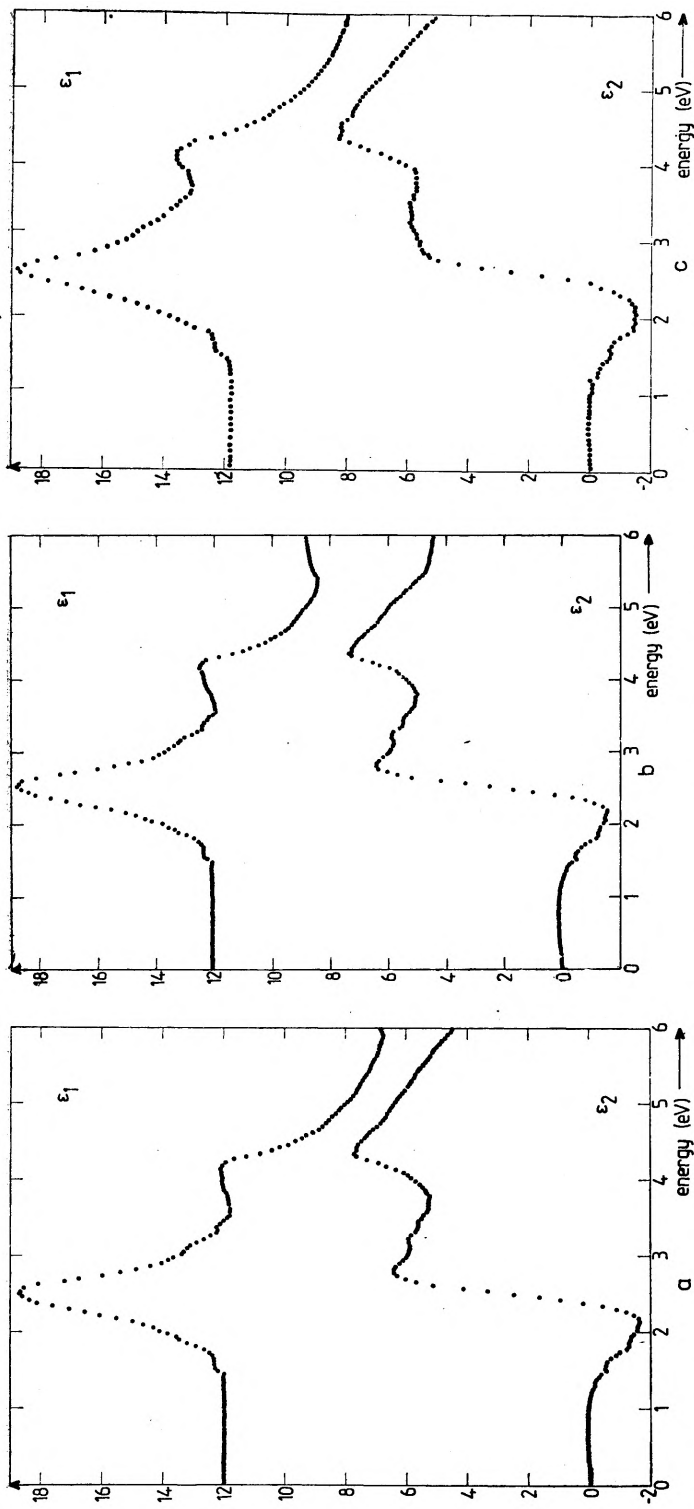


Fig. 4. Real and imaginary parts of the complex dielectric constant for  $Zn_3P_2$  calculated on the base of (a) Philipp-Taft method, (b) SKK method, and (c) "power series" method

The same results of measurements have been exploited in calculations, as those used in the Section 3.1. It should be noticed that no extrapolation outside the measurement range was required. The calculated values are presented in Fig. 4b.

### 3.3. Calculations by the method of "power series"

The formulae like those used in the method due to Philipp-Taft were exploited in the calculations with the modified extrapolation outside the final point, according to the formula

$$R(E) = a_0 f(E) \left( \frac{E}{E_b} \right)^{-4}, \quad (6)$$

which may be easily transformed to yield the form (used in calculations)

$$\ln R(E) = \sum_{m=1}^{\infty} a_{2m} \left( \frac{E_b}{E} \right)^{2m} + \ln \left[ a_0 \left( \frac{E}{E_b} \right)^{-4} \right]. \quad (7)$$

Calculations were carried out by exploiting the experimental results used in Sections 3.1 and 3.2 and assuming the zeroing condition for  $\Theta(E)$  at the points  $E = 0.10$  eV and 1.00 eV. The results of calculations are shown in Fig. 4c.

### 3.4. Discussion of results of calculations

The figures allow to state the similarity of shape of functions  $\varepsilon_1(E)$  and  $\varepsilon_2(E)$ , received by different calculation methods. Also, the numerical values of real and imaginary parts of dielectric permittivity are very close to each others. In [11] the values of refractive index in the vicinity of oblique energy gap,  $n_i = 3.49$ , and in the vicinity of the direct energy gap,  $n_d = 3.59$  have been determined. The obtained values of the refractive index  $n_i = 3.47$  and  $n_d = 3.49$  remain in good agreement with the values given above. The refractive index reaches its maximal value 4.34 for energy 2.54 eV, and maximal value 4.15 for energy 3.81. In the transparency region it is practically constant and reaches the value 3.47. Also, the real part of the dielectric permittivity is constant within this region and amounts to 12.05.

The fact that the maxima of the dependence  $\varepsilon_2(E)$  lie in the vicinity of the maxima of the reflection spectrum  $R(E)$  speaks for the correctness of the results obtained. The dependence  $\varepsilon_2(E)$  has two distinct maxima, the values of which are 6.4 for energy 2.82 eV, and of 7.6 for the energy 4.34 eV, as well as two less distinct structures for energies 3.2 and 3.45 eV. It is worth mentioning that the values of  $\varepsilon_2(E)$  are close to zero in the transparency region, which is consistent with the general requirement (see [1]). There, the non-physical behaviour of  $\varepsilon_2(E)$  in the vicinity of 2 eV (Fig. 4) may not be avoided. Along the 1.14–2.38 eV segment  $\varepsilon_2(E)$  has negative values creating a nonphysical dip. Similar situation was obtained in the calculations for AgCl presented in paper [16]. The authors of the last paper carried out a fundamental analysis of the used method of calculations (which was the Philipp-Taft method) and stated that the erroneous results of the reflection coefficient measurements were the only source of nonphysical dip in the vicinity of

$E_g$ . They have also shown that it can be liquidated by correction of these results in the region where the dip appears. It may be suspected that also in our calculations the appearance of the dip is (at least partially) caused by the errors in measurement results. This, may be also caused by improper „sewing” of the measurement data with those from the literature.

#### 4. Optical constants of $Zn_3As_2$

Similarly, as it was the case for  $Zn_3P_2$ , the compound  $Zn_3As_2$  is a semiconductor of p-type [2]. The concentration of holes at the room temperature is of order of  $10^{23} \text{ m}^{-3}$ , while the mobility is of order of  $10^{-3} \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$ . The value of the energy gap  $Zn_3As_2$  obtained from the absorption measurement amounts to 0.99 eV at 300 K [12]. The atomic concentration of  $Zn_3As_2$ , necessary to calculate the effective number of electrons, has been determined in the work [13] on the base of the given density of  $Zn_3As_2$ . It amounts to  $0.49 \cdot 10^{29} \text{ m}^{-3}$ .

The calculations of optical constants of  $Zn_3As_2$  have been performed by using two methods: that of Philipp-Taft and the SKK method, as it was the case for  $Zn_3P_2$ .

##### 4.1. Calculations by using the Philipp-Taft method

The calculations with the help of this method were based on our own results obtained from the measurement of the reflection coefficient spectrum for  $Zn_3As_2$  for one of the samples (No. RA-2). These measurements were completed up to 30 eV with the results reported in the works [4, 14]. Fitting of these results appeared to be much difficult, since the results given in the work [4] exceeded our data by about 20%, while those reported in [14] were, in turn, less than the data reported in the work [4] by about 70%. Despite a rather “smooth sewing” performed for all the three fragments of the reflection coefficient spectrum, the effect of uncomplete fitting of the data is visible in the results of calculations.

In the course of calculations it appeared impossible to perform the fitting of  $\theta(E)$  to zero (in the least-square sense) below the value  $E_g$  for physically justified assumption that  $A \leq 0$ , where  $A$  is the exponent from the extrapolations (formula (1)). The immediate reason for which the said fitting could not be performed was that the sum of  $\theta_1(E) + \theta_2(E)$  for the exploited data of the reflection coefficient of  $Zn_3As_2$  was greater than zero in the region of transparency. The fitting for unchanged data of  $R(E)$  would be possible solely by accepting the nonphysical course of the curve extrapolating the coefficient of reflection above the upper measurement limit, i.e., by assuming  $A > 0$ . Of course, such a solution is unacceptable.

The described above behaviour of the sum  $\theta_1(E) + \theta_2(E)$  was to the highest degree due to the lack of the measurement of  $R(E)$  in the transparency region, where the extrapolation  $R(E) = \text{const}$  was applied. The last manipulation is probably responsible for the high value of the coefficient of reflection in this region. It could be also due to the difficulties of compiling the literature data and those obtained in our own measurements with the data available for us. However, the latter reason could not be eliminated since



the broad range of the reflection coefficient is the basic condition for application of Philipp-Taft method. An attempt to complete the spectrum of reflection coefficient of  $Zn_3As_2$  from the low energy side by employing the Leveque method (see [1]) has failed, so far.

#### 4.2. Calculations by using the SKK method

Similarly, as it was the case with Philipp-Taft method, the basis for the calculations in the SKK method the measurements of the reflection coefficient of  $Zn_3As_2$  for the sample RA-2 created. When the SKK method (see part II in [1]) was used the measurements were not completed with the literature data.

In the calculations we have used the data of  $R(E)$  read out each 0.01 eV. The results of these calculations are shown in Fig. 5.

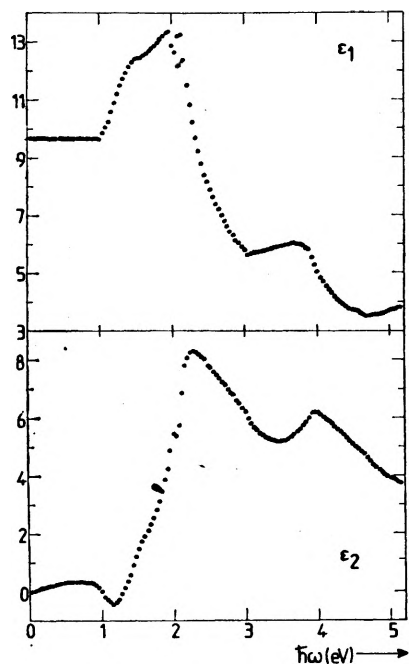


Fig. 5. Real and imaginary parts of the complex dielectric constant of  $Zn_3As_2$  calculated by the SKK method

As it may be seen the graphs,  $\epsilon_1(E)$  and  $\epsilon_2(E)$  have two distinct maxima at the vicinity of energies 2.0 eV and 4.0 eV. Certain singularities may be also observed for the energies of about 1.4 eV. The first maximum is split both for  $\epsilon_1(E)$  and  $\epsilon_2(E)$ . In the first case the maxima are noted for 1.95 eV and 2.15 eV, while for  $\epsilon_2(E)$  the maxima occur for 2.0 eV and 2.25 eV. Also a maximum in the plot may be observed for  $\epsilon_1(E)$  at 3.70 eV and for  $\epsilon_2(E)$  at 3.95 eV. The same qualitative agreement may be stated between the obtained results and the run of reflection coefficient for  $Zn_3As_2$ , discussed in the work [11].

#### 5. Final remarks

This work reports the steps made by us in order to recognize and apply the calculation methods of optical constants in semiconductors with the help of the Kramers-Kronig relations. Our work is partly a review, which may, at least partly, fill the gap existing in

the world literature devoted to the calculations of optical constants. While discussing the particular methods we tried to derive all the basic dependences, as in most cases they are neglected in the literature.

The further methodological improvement of numerical calculations of the contribution to  $\Theta$  coming from the measurement range, i.e.,  $\Theta_2$ , as well as the further perfecting of the estimation procedure used to determine the error introduced by the method seem advisable. The reflection spectrum being given in a discrete form due to specificity of the measurements their results should be used immediately as the data to the programme, while the error of the calculation of  $\Theta_2$  should depend mainly on the measurement density. The very complex problem of estimating the errors caused by the choice of the concrete extrapolation method has not been finally solved either. The available literature does not present even the rough attempts to assess this error. Thus, it seems necessary to verify practically the methods based on modified extrapolation due to Philipp-Taft. Theoretically, their application may give good results. The same refers to the methods not requiring the extrapolation, as the SKK method, for instance. On the one hand, their application is connected with some complications of calculation, on the other hand, however, the fact that they do not require any knowledge of the reflection coefficient outside the measurement interval seems to be advantageous. The SKK method gives the good results only in the case when the measurements of  $R(E)$  are restricted to the transparency region in semiconductor or the absorption value outside this region is known. However, this last possibility is realized very rarely. Next step in improving the SKK method would be to elaborate the programme, which would perform the self-consistent calculations by using Leveque method in order to complete the reflection coefficient spectrum from the low energy side on the base of the absorption measurements available in this range. All these attempts should be undertaken to achieve the final goal, i.e., to write the programme according to which the optical constants should be calculated for an arbitrary semiconductor, for which the reflection coefficient is known in its arbitrary range. Of course, the error of the calculated optical constants should be also determined. It seems, that this final programme should be based simultaneously on several independent methods of optical constant calculation.

Summing up, it may be stated that both the Philipp-Taft method and the SKK method proved to be not easily applied to  $Zn_3As_2$  and  $Zn_3P_2$ . First of those methods requires a large measurement range, while the other – a high accuracy of the reflection coefficient measurement. This explains the fact that the SKK method is used rarely, since, as a rule, it is easier to broaden the measurement range than to increase sufficiently their accuracy. It should be also emphasized that the results given in this work are only the first approximation of the run of the optical constants both for  $Zn_3As_2$  and  $Zn_3P_2$ . The calculations aiming to obtain the accurate values of the optical constants of the said compounds are continued.

Actually, the results of calculations of  $\varepsilon_1(E)$  and  $\varepsilon_2(E)$  obtained both for  $Zn_3P_2$  and  $Zn_3As_2$  cannot be interpreted on the base of energy structure calculations for these semiconductors. As it has been shown in [11, 15] the characteristic energies of the reflection spectrum are not consistent either with the unique model of the energy structure of  $Zn_3P_2$  and  $Zn_3As_2$ , known till now [17].

In order to recognize more accurately the optical constants for  $Zn_3P_2$  and  $Zn_3As_2$  further measurements of the absolute value of the reflection coefficient are indispensable. Here, both the room temperature and the low temperature measurements are important. In order to point out the anisotropic properties of  $Zn_3P_2$  and  $Zn_3As_2$  the measurements of the reflection coefficient for the polarized light made on oriented samples may be used. Such measurements are being made in our laboratory.

*Acknowledgements* – The authors are deeply indebted to Mrs. B. Sujak-Cyrul and Mr. J. Wróbel for the help in the reflection coefficient measurement. This work is partly based on the thesis for master degree of two of us (K. J. and J. W.).

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*Received January 25, 1981*

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

**Часть V. Оптические константы  $Zn_3As_2$  и  $Zn_3P_2$**

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 работы в дополнительных направлениях, описанных в трёх первых частях.

В первой части представлен критический анализ применяемых до настоящего времени методов расчёта, основанных на дисперсионных соотношениях Крамерса-Кронига. Обсуждены также методы расчётов 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 расчётов подробно проводится в IV части.

Настоящая (v) часть содержит результаты расчёта для  $Zn_3As_2$  и  $Zn_3P_2$ , произведённых с помощью усовершенствованных методов, а также на основе наших результатов измерений. Произведены измерения коэффициента отражения при температуре 300 К, в неполяризованном свете, а также рассчитаны и обсуждены спектральные характеристики действительной и мнимой частей комплексной диэлектрической постоянной обоих полупроводников.