Calculation of Transmission Coefficient of Bismuth Planar Waveguide in Magnetic Field in the Far Infrared Range

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INTRODUCTION

The paper aims to study the behavior of a system consisting of a planar waveguide made of bismuth and located in a magnetic field. The electromagnetic wave is propagating through a waveguide whose walls are made from anisotropic monocrystal. Passage through the planar waveguide of a laser radiation leads to cyclotron absorption of electromagnetic radiation. The quality of a crystals and value of $k_B T$=0.36 meV permit to observe cyclotron resonances and dielectric anomalies of electrons and holes in *L* and *T* points of the Brillouin zone. A convenient physical model and a mathematical model are provided where a classical point of view is considered by the use of Maxwell's equations to model the propagation of electromagnetic wave. Newton's method was used to solve the characteristic equations in complex plane. The complete algorithm for calculation of the shapeline of the magnetooptical experiment in far infrared range of spectrum is submitted.

Keywords: anisotropic monocrystal, planar waveguide, infrared radiation, transmittance.

BACKGROUND

Compounds based on bismuth and antimony are widely used in the creation of thermoelectric devices and appear promising for use in optoelectronics. Extensive opportunities are opening up when using semimetals as materials for creating effective receivers and modulators of radiation operating in the far infrared region of the spectrum [8,10,11]. The solution of such problems requires detailed information about the band structure and the influence of various external influences: temperature, pressure, magnetic field on the energy spectrum of charge carriers.

It is known that resonance, and especially oscillation effects, are the most accurate and most direct methods of studying the band structure of solids.

Experimental observation of oscillation effects in bismuth provides the greatest amount of unique information about this material. The anisotropy of the properties of the object under study and the small values of the effective cyclotron masses of the charge carriers allow measurements to be made in experimentally achievable magnetic fields. Calculation methods using known models provide extensive information.

The shape of the Fermi surfaces of bismuth has been fully restored by methods of cyclotron absorption and magnetoresistance oscillations (Shubnikov-De Haas effect). Precise measurements of microwave absorption [1-4] give the values of cyclotron masses both for electrons and holes as well as the exact orientation of isoenergetic surfaces with respect to the crystallographic axes in bismuth at the boiling temperature of liquid helium.

In [12,13] the results of studies of bismuth monocrystal in the region of plasma reflection edge are presented. The experiment was based on the mechanism of spin-polarized magneto-optical current generation of relativistic electrons described by the Dirac equation in bismuth-type crystals [5].

Experimental measurements were performed in a quantized magnetic field in Faraday geometry. Along with the reflection, the rotation angle of the polarization plane (polar Kerr effect) was measured [12,13]. High-frequency conductivity modeling was performed for right- and left-hand circularly polarized photons. It was found that intraband transitions of electrons involving Landau levels with n=0 are possible only for photons with one of two possible circular polarizations and electrons with spin +1/2. Consideration was carried out in magnetic fields up to 7 Tl and in the range of photon energies from 2 to 87 meV. In [12,13] the "experimental" high-frequency conductivity obtained from the Fourier transform and generalized magneto-optical Kramers-Kronig analysis (MOKKA) of reflection spectra were compared with the theoretical high-frequency conductivity, within the framework of high-frequency conductivity modeling using the Kubo formula. At the same time in [12,13] there is no comparison of simulation results with experimental reflection spectra and no discussion of the influence of variation of electronic spectrum parameters on the form of the simulated reflection coefficient.

MAIN FOCUS OF THE ARTICLE

In this paper, an attempt is made, by the method of mathematical modeling of physical processes, to extract information from the results of a physical experiment, which cannot be obtained from the experimental material by a direct method. The physical experiment simulated in this work belongs to the class of quantum oscillation effects. De Haas - van Alphen effect, Shubnikov - de Haas effect, magnetostriction oscillations and magneto-optical oscillations in the study of the band structure of solids give the most extensive information on the subject of research. However, their interpretation, with the exception, perhaps, of the de Haas - van Alphen effect requires a comprehensive mathematical processing of the experimental results.

The peculiarity of the considered approach in modeling the results of a physical experiment is an attempt to take into account all the data obtained during the experiment. The digital recording of the experimental results allows one to obtain data arrays containing up to 2000 values in a single magneto-optical spectrum. However, the processing of the results of such an experiment, which is accepted in solid state physics, takes into account only the field positions of the oscillation minima, which is less than 0.5 percent of the experimental information obtained. Therefore, it would be realistic to expect that, as a result of modeling the shape of the magneto-optical spectrum, one could check the applicability of the available physical models, select the optimal one, and obtain substantially new information about the subject of the study.

Problem formulation

There is a problem of investigation of a signal passing through a planar wave guide in magnetic field (Fig. 1). A laser radiation is passed through two parallel anisotropic crystals made from bismuth. The two crystals, with walls well polished, are placed in the magnetic field, at constant temperature; both parts constitute a planar waveguide. There is interaction of radiation with the walls of a planar waveguide.

Classically the problem is modeled using Maxwell equations where the medium effect on the propagation of the electromagnetic wave is taken into account by the permittivity tensor composed of nine components. The effective mass of bismuth in magnetic field is a tensor of nine components. The relaxation time is also highly dependent from the magnetic induction. The analysis and interpretation are done in terms of the dependence of the radiation intensity in function of the magnetic induction given by the transmittance coefficient. It is required to lead analysis when the vector of the induction magnetic field is directed along bismuth high symmetry directions i. e., the crystallographic axis, mainly along the binary, bisectrix and trigonal directions (Fig. 2).

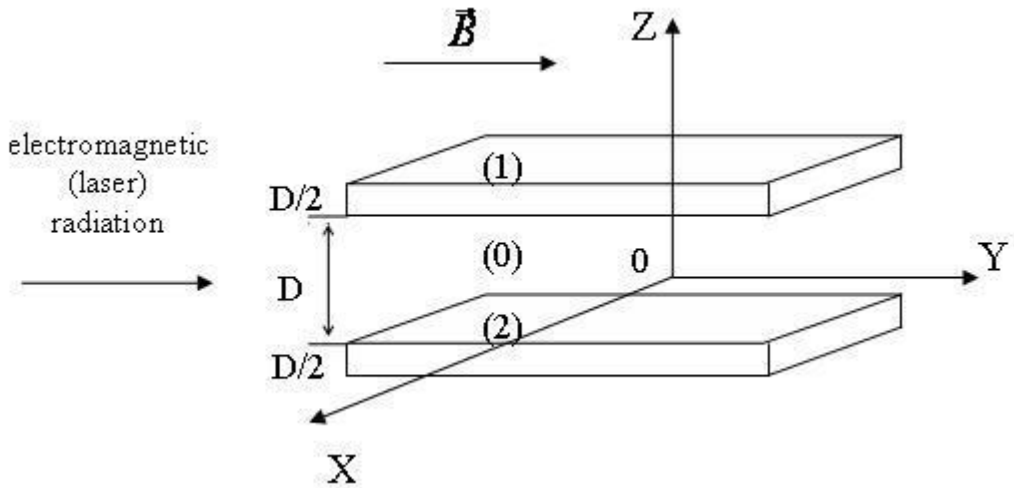


Figure 1. Planar waveguide together with orientations of electromagnetic wave and magnetic field induction

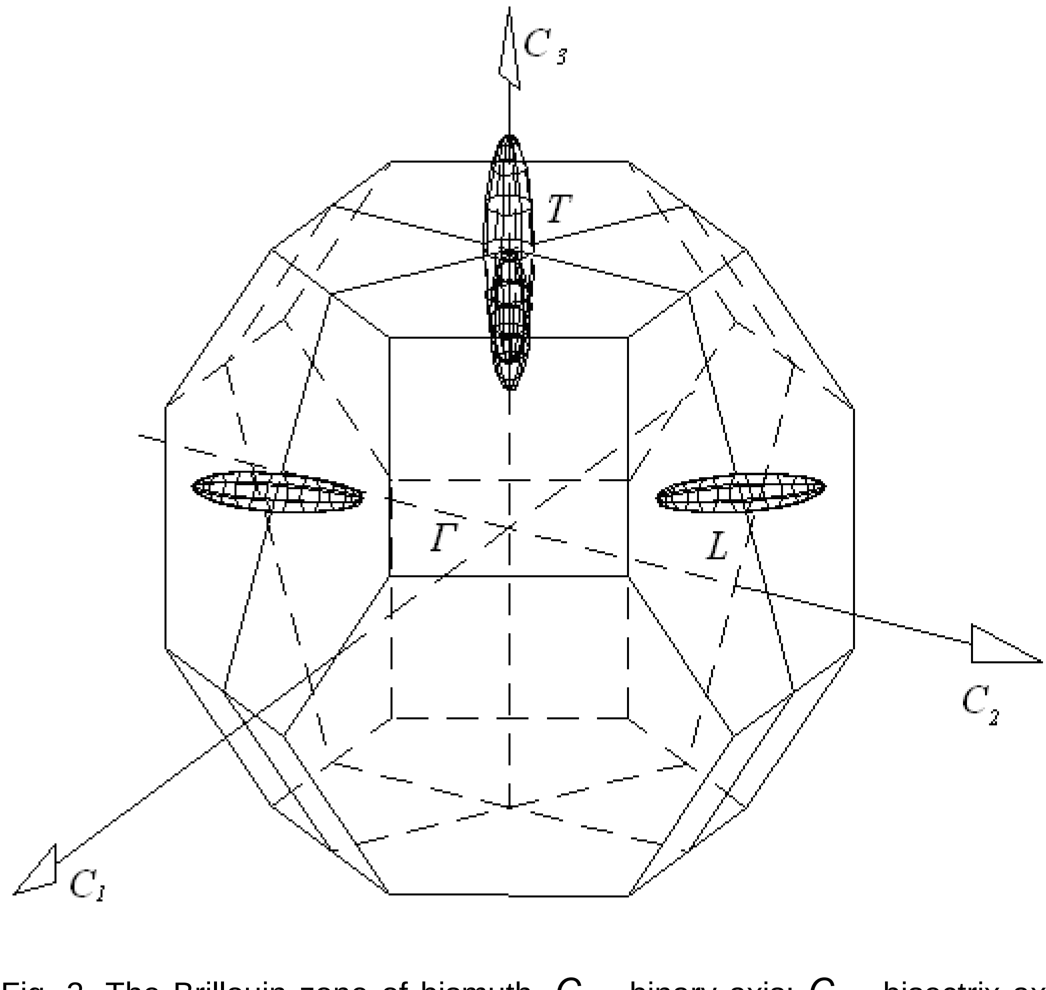


Fig. 2. The Brillouin zone of bismuth. C_1 - binary axis; C_2 - bisectrix axis; C_3 - trigonal axis; Γ - center of Brillouin zone; L - point of localization of electronic extremums; T - point of localization of hole extremum.

View the complexity of the problem, analytic method together with numerical method and computing techniques are applied.

Solution of the Maxwell equations

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad (1)$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{j}, \quad (2)$$

$$\vec{\nabla}\vec{B} = 0, \quad (3)$$

$$\vec{\nabla}\vec{D} = \rho, \quad (4)$$

with material relations:

$$\vec{D} = \hat{\varepsilon}\varepsilon_0 \vec{E}, \quad (5)$$

$$\vec{B} = \mu\mu_0 \vec{H}, \quad (6)$$

look like [9]:

$$\vec{E} = \vec{E}^{(1)} exp(-\alpha z) exp(i(\omega t - q_y y)), \quad (7)$$

Where $\vec{E}$ - the electric field strength of electromagnetic wave, ω - circular frequency of electromagnetic wave, α - the transverse, wave number, q_y - the longitudinal wave number as arranged in fig. 1, and the coefficient $^{(1)}$ has been used, to express that the complex amplitude falls into medium (1) fig. 1.

A solution of a wave equation for empty space (0) (fig. 1) is searched as:

$$\vec{E}^{(o)} = \vec{E}^{(o)} \exp(-\alpha_0 z) \exp(i(\omega t - q_y y)). \quad (8)$$

In calculations it is convenient to compare energy $W(B)$, transferred by a wave at some value of the magnetic field B, to energy $W(0)$, transferred by the wave at $B = 0$, that is the transmittance of a planar wave guide is determined as

$$T(B) = \frac{W(B)}{W(0)}. \quad (9)$$

After taking into account boundary conditions next and numerical evaluations of parameters the expression for the transmittance $T(B)$ (4) takes a form [7]:

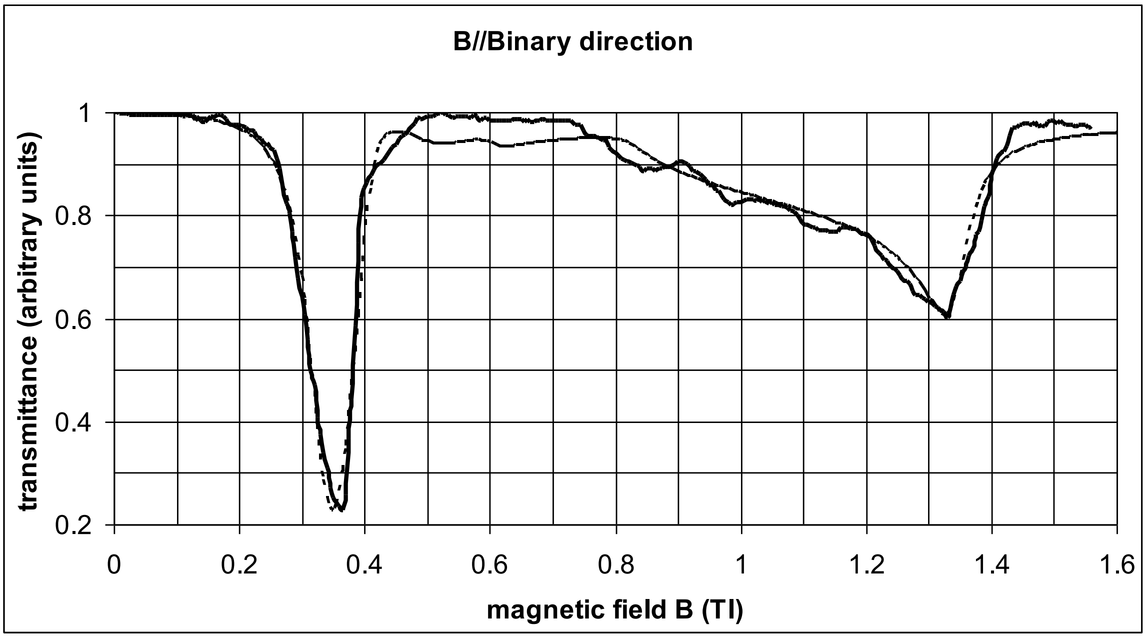
$$T(B) = 1.055 \times exp\{2L[q''_y(B) - q''_y(0)]\}. \quad (10)$$

Numerical results when the magnetic field is oriented along the binary axis

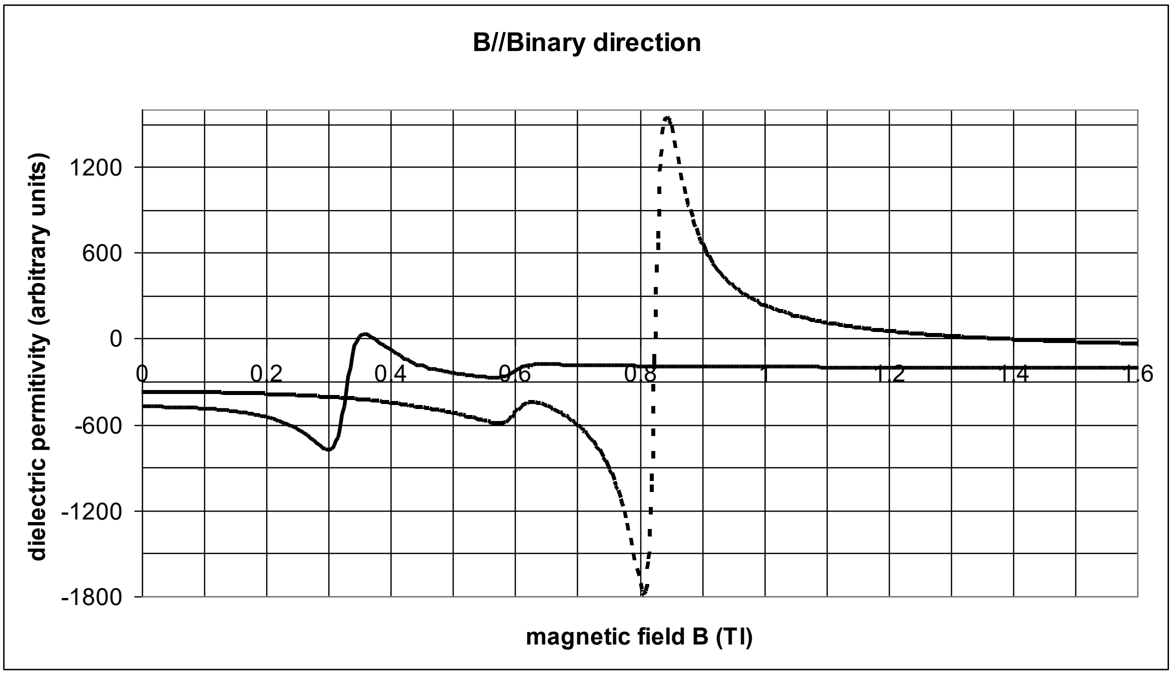
On the fig. 3, we present the results of modeling (solid line) of the form of line of the magnetooptical experiment (dashed line) when the magnetic field is oriented along the binary axis.

When the vector of the magnetic field is parallel to the binary axis there are three kinds of charge careers (fig.2). These are the electrons with effective masses different 10 times each other, and holes with intermediate effective masses. In consistent with band structure of bismuth and results of numerical experiment we determined that there are signal from electrons with the smallest effective masses and holes. Valley at

B=0.35 Tl (Fig. 3a) is the signal from light electrons and valley at B=0.132 Tl is the signal from holes. In numerical experiment we canceled consecutively other members of the components of high frequency conductivity tensor. Computations permit us to draw conclusion that we can not see signal from electrons with largest effective masses.



a)



b)

Fig. 3. Results of modeling of the form line of the magnetooptical experiment when the magnetic field is oriented along the binary axis. a) experimental results (solid line) and the best fitting (dashed line), b) real parts of a dielectric functions for ordinary (solid line) and extraordinary (dashed line) waves.

Explanation of the experimental results consists in the view of solution (7) of Maxwell equations (1-4). Coefficients α and q_y are the components of the wave vector of the electromagnetic wave passing through the walls of the planar waveguide. Coefficients α and q_y are complex numbers, which we can get in the result of numerical procedure. In all range of the experimental magnetic field $\alpha >> q_y$. It means that, the wave vector of the electromagnetic wave is directed to the z axis (fig. 1) in our coordinate system. Thus the electromagnetic waves are spreading in the direction perpendicular to the magnetic induction vector. These waves we can classify in the ordinary and extraordinary waves. These waves are like the ordinary and extraordinary waves in the birefringence phenomena in crystallooptics. Ordinary wave is polarized in the direction of the magnetic field and it is clear transversal electromagnetic wave. Extraordinary wave is polarized in the XZ plane and it is transversal-longitudinal wave.

From the general theory for these waves the dielectric permittivity for ordinary wave

$$\varepsilon_o = \varepsilon_{yy} \tag{11}$$

and for extraordinary wave

$$\varepsilon_e = \varepsilon_{xx} - \varepsilon_{xz} \cdot \varepsilon_{zx} / \varepsilon_{zz} . \tag{12}$$

Were ε_{ij} - components high frequency dielectric permittivity tensor.

On the fig 3b there are graphs of the real parts ε_o and ε_e. When the real part of the dielectric permittivity is negative, electromagnetic wave can not propagate in the substance and all the power is reflected from the surface of the crystals. In result the coefficient of transmission is equal to 1. At the point where the dielectric permittivity becomes zero, we have the cyclotron resonance. The energy is absorbed by electron subsystem of the crystal and the transmission coefficient is therefore decreasing. At the range of the magnetic field where the dielectric permittivity is positive the transmission coefficient is less than 1. The dielectric function is decreasing after it has reached its maximum. The point where the dielectric permittivity becomes zero is called dielectric anomaly. Before this point the dielectric function is negative and the electromagnetic wave is reflected from surface of the crystal.

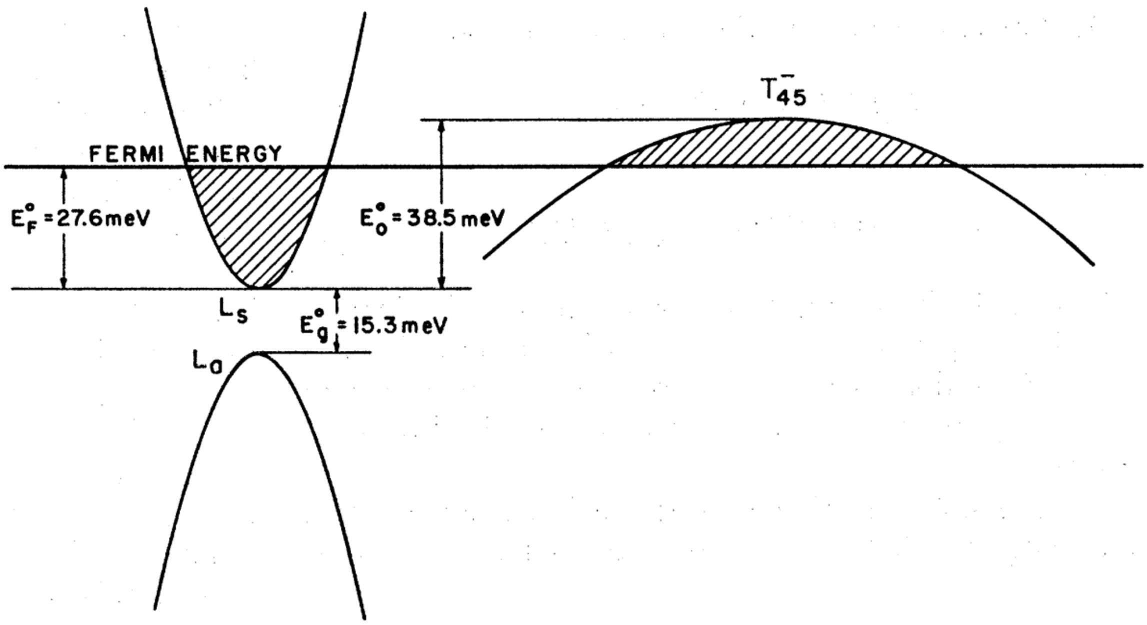


Fig. 4. Energy diagram of bismuth [6].

In reality we have superposition of these processes for ordinary and extraordinary waves. After summation they must give experimental picture. But the reality of modeling is far from this relatively easy and clear picture.

The subtle of our modeling experiment consists in that we varied charge carrier densities, relaxation time and lattice dielectric permittivity with increasing magnetic field. We have physical reasons for justification of this procedure. The Fermi level is arranged on 27.6 meV higher the bottom of the conduction band (Fig. 4).

Quantum of electromagnetic radiation can excite only small part of the conduction band electrons. But in the expressions for conductivity tensor the true value for electron concentration is figured. It means that in fitting theoretical results to experimental, the charge carrier density must be a variable parameter. Moreover, charge carrier density can differ from extremum to extremum. The reason for this is very easy. For given direction of magnetic field the curvature in the plane perpendicular to the vector magnetic induction does not equal each other for others constant energy surfaces. It means that there are different densities of the electronic levels for other extremums. Thus different numbers of electrons will be excited from other surfaces of constant energy. In result charge carrier density will be different for other surfaces of constant energy.

Relaxation time and lattice dielectric permittivity also generally speaking depend from the nature of the constant energy surface and the location of the constant energy surface with respect to the direction of the magnetic field. It is physical reason, why we can vary these parameters.

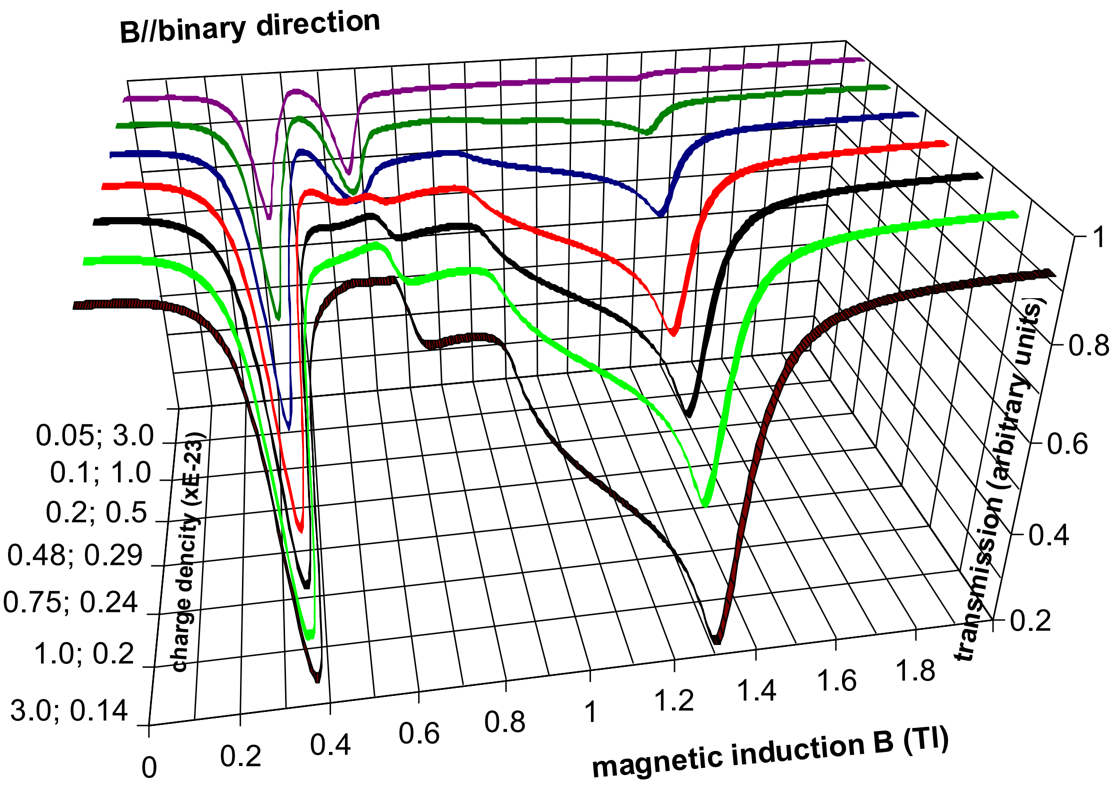


Fig. 5. Results of modeling of the form line of the magnetooptical experiment when the magnetic field is oriented along binary axis: a) $n_e=0.05x10^{23}$ m^{-3}, $n_h=3.0x10^{23}$ m^{-3}; b) $n_e=0.1x10^{23}$ m^{-3}, $n_h=1.0x10^{23}$ m^{-3}; c) $n_e=0.2x10^{23}$ m^{-3}, $n_h=0.5x10^{23}$ m^{-3}; d) $n_e=0.48x10^{23}$ m^{-3}, $n_h=0.29x10^{23}$ m^{-3} (the best fitting); e) $n_e=0.75x10^{23}$ m^{-3}, $n_h=0.24x10^{23}$ m^{-3}; i) $n_e=1.0x10^{23}$ m^{-3}, $n_h=0.2x10^{23}$ m^{-3}; j) $n_e=3.0x10^{23}$ m^{-3}, $n_h=0.14x10^{23}$ m^{-3}; n_e, n_h - charge carrier density for electrons and holes.

At the fig. 5 we submit results of modeling of the form of line of the magnetooptical experiment, when the magnetic field is oriented along the binary axis.

Charge densities of electrons and holes are variable parameters. Charge densities of electrons increase from n_e=0.05x10^{23} cm^{-3} to n_e=3.0x10^{23} cm^{-3}, charge densities of holes decreases from n_h=3.0x10^{23} cm^{-3}to n_h=0.14x10^{23} cm^{-3}. Value n_e= n_h=3.0x10^{23} cm^{-3} corresponds the real value of charge density at T=4.2 K. At increasing charge density of electrons the depth of a valley at B=0.36 Tl is increasing, and at increasing charge density of holes the depth of a valley at B=1.32 Tl is decreasing. Explanation of this behavior for electrons consists in that at decreasing concentration of electrons absorption is decreasing also. There is the best fitting at n_e=0.48x10^{23} cm^{-3}, n_h=0.29x10^{23} cm^{-3}.

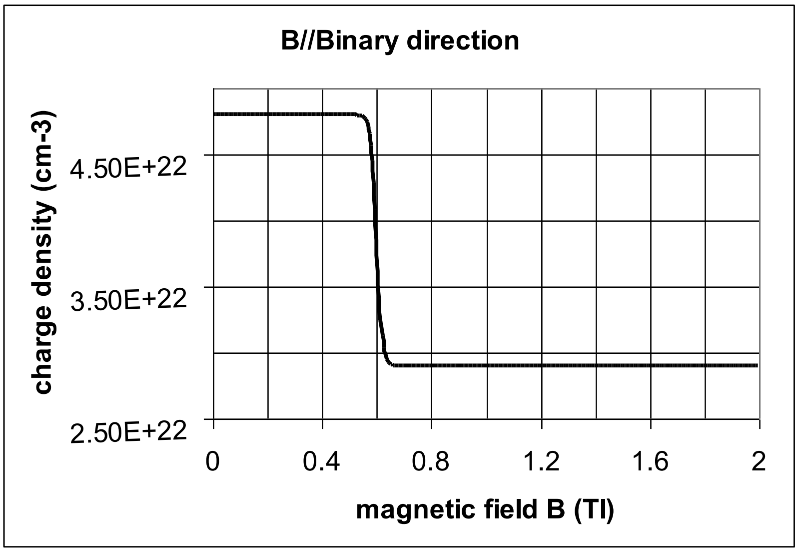


Fig. 6. Modeling of charge densities for electrons and holes.

The dependence of charge densities for electrons and holes from magnetic field is submited on the fig 6. The position of step in this dependence is at B=0,6Tl.

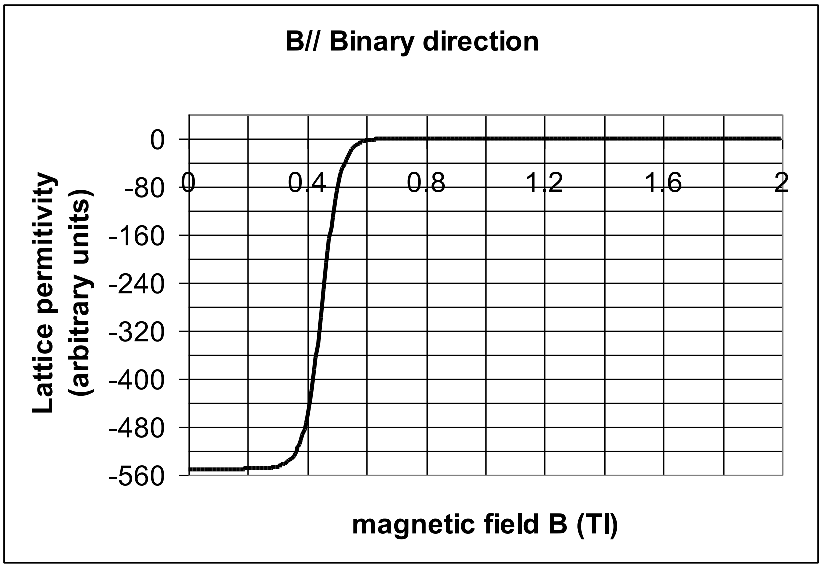


Fig. 7. Modeling of the lattice dielectric permittivity for electrons and holes.

Modeling of the lattice dielectric permittivity for electrons and holes (Fig. 7) showed, that the best fitting there is when there is one value of the lattice dielectric permittivity for electrons and an other for holes.

Numerical calculations can come to errors or to mistakes in determination of the roots of the dispersion equation. We have used Newton method to solve the transcendental equation on complex plane with complex solutions. The sensitivity of the results of numerical calculations to initial guess of solution permits us to form an opinion about stability of the solution and indirectly about correctness of our numerical procedure.

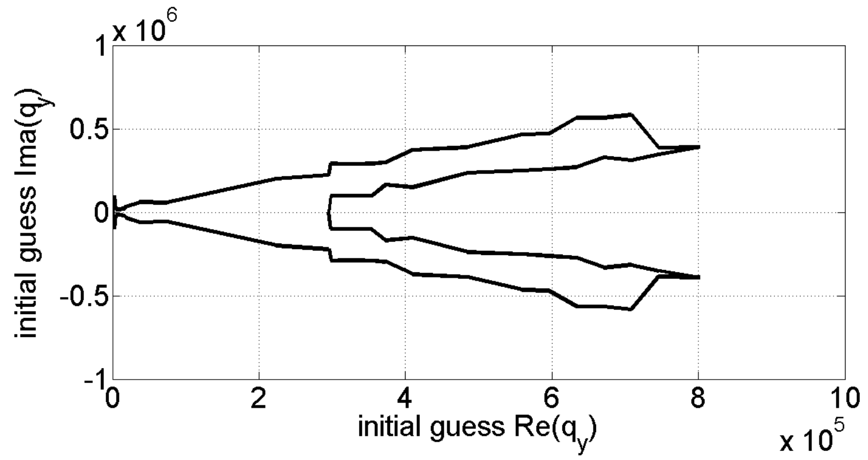


Fig. 8. Area of stability relative to initial guess of solution.

The initial guess of solution is complex number ($k_o = \frac{2 \cdot \pi}{\lambda} = 1{,}98 \cdot 10^4$ m^{-1}, 0). We can see from fig 8, that area of stability of solutions of the dispersion equation relative to initial guess of solution exceeds all reasonable suggestions.

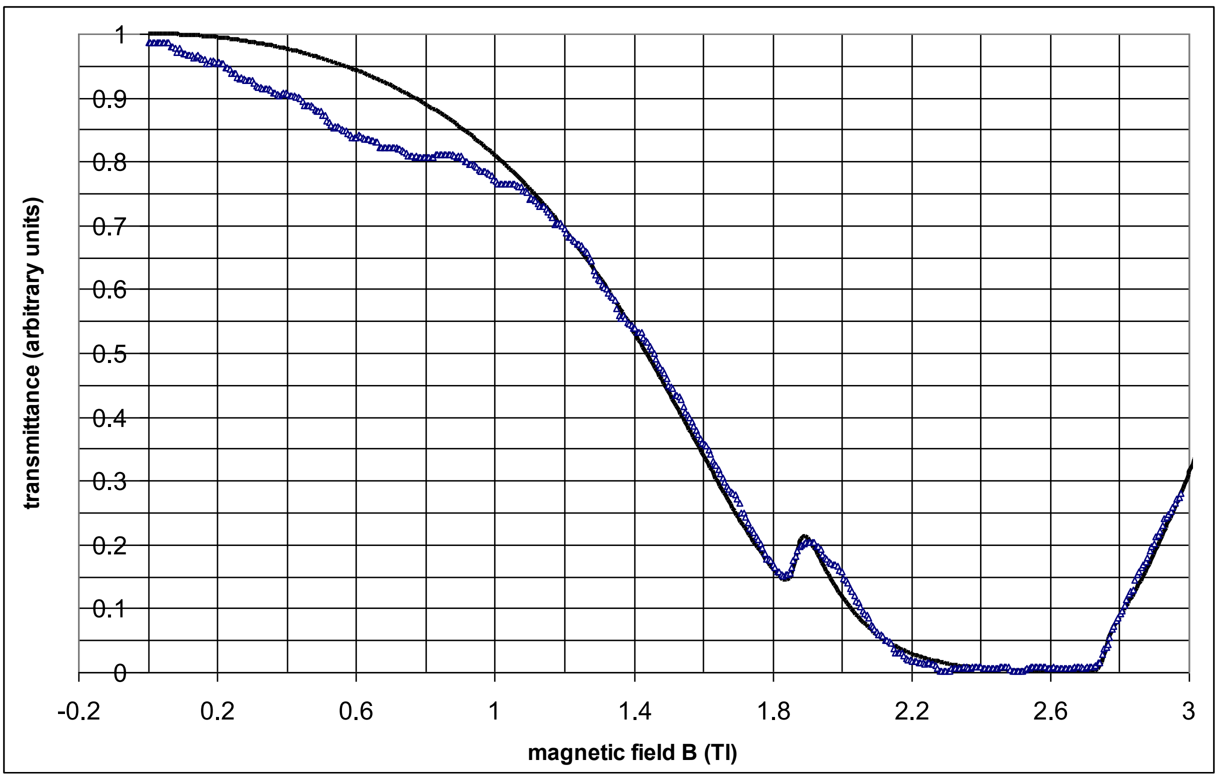


Fig. 9. Results of modeling of the form of line of the magnetooptical experiment when the magnetic field is oriented along trigonal axis.

Numerical results when the magnetic field is oriented parallel the trigonal direction

On the fig. 9 we present the results of modeling (solid line) of the form of line of the magnetooptical experiment (triangles) which is the best fitting of the experimental results when the magnetic field is oriented along trigonal axis (fig. 2).

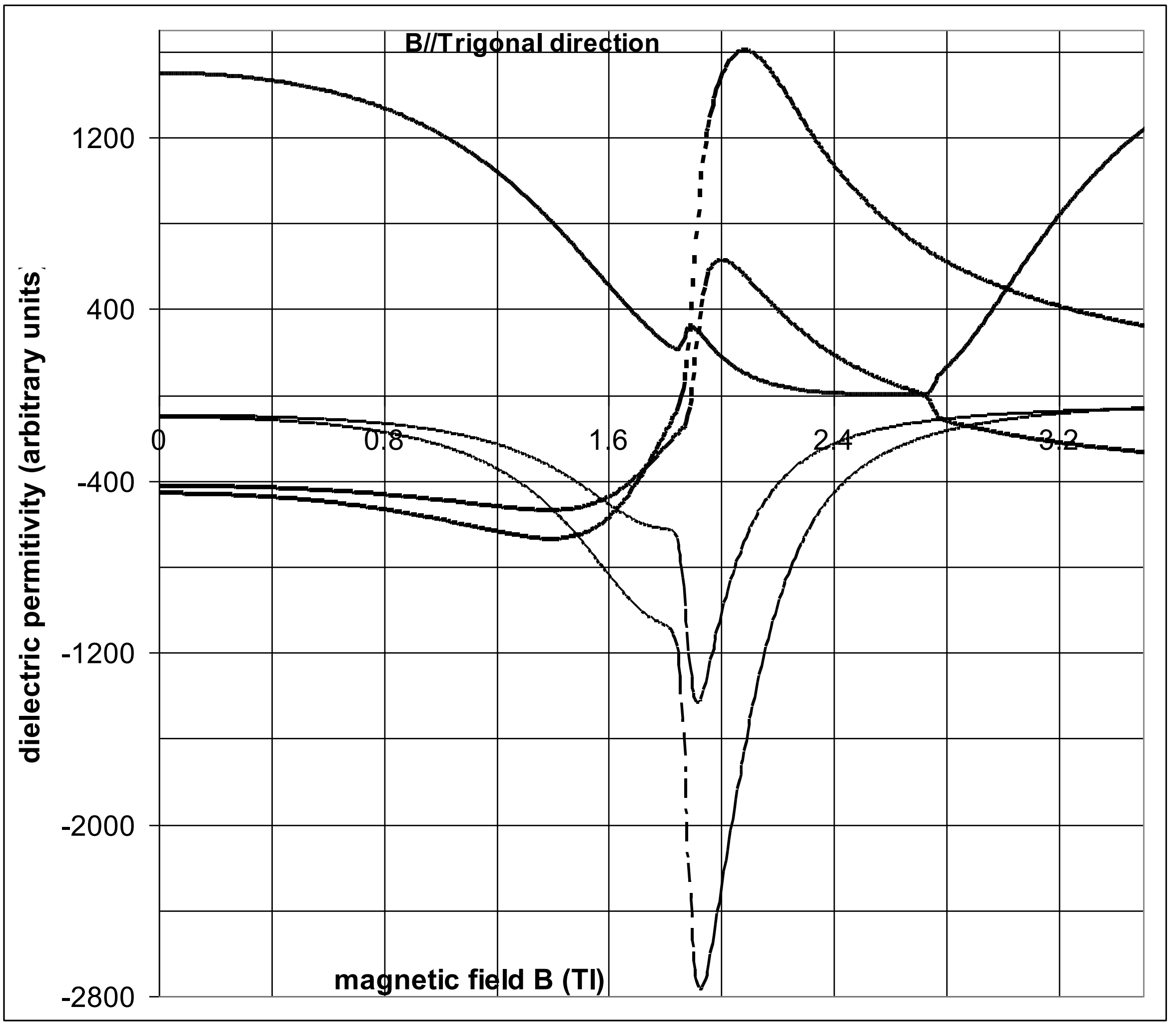


Fig. 10. Results of modeling of the form of line of the magnetooptical experiment when the magnetic field is oriented parallel the trigonal axis: the best fitting (solid line) and real (dashed lines) and imagine (dashed-point lines) parts of a dielectric functions for ordinary (lower intensity) and extraordinary (greater intensity) Voigt waves.

When the vector of the magnetic field is parallel to the trigonal axis there are two kinds of charge careers. It is electrons and holes. The cyclotron mass of electrons is less than cyclotron mass of holes. This defines the more importance of electrons for this relative configuration vector of magnetic induction and crystallographic directions.

We can observe (fig. 10), that the reduction of the intensity coincides with decrease of the imagine part of the dielectric function for ordinary and extraordinary waves. Local maximum at B=1.91 Tl appears when the real part of the dielectric function has maximum derivative with respect to magnetic induction. Strictly speaking it is the condition for the occurrence of resonance. We had taken the numerical derivatives of the real parts of a dielectric function for ordinary and extraordinary Voigt waves. The field position the maximum of the derivative for extraordinary wave coincides with the field position the local maximum of transmittance.

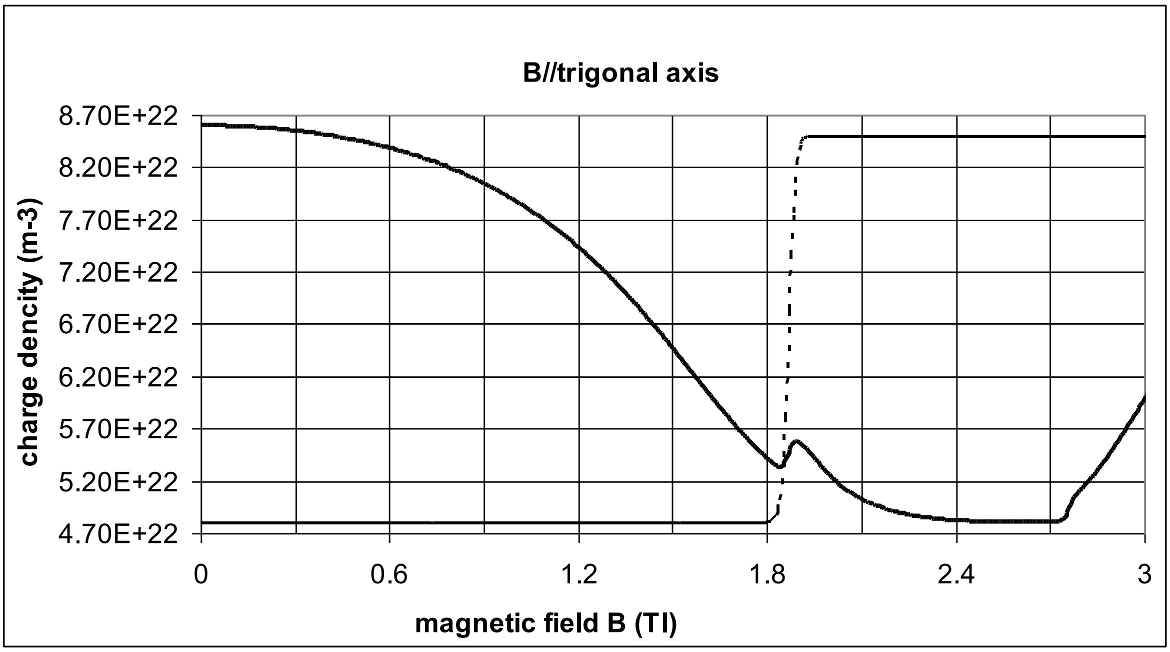


Fig. 11. Results of modeling of charge density (dashed line) dependence from magnetic field and the form line of the magnetooptical experiment (not in scale) when the magnetic field is oriented parallel the trigonal axis (solid line).

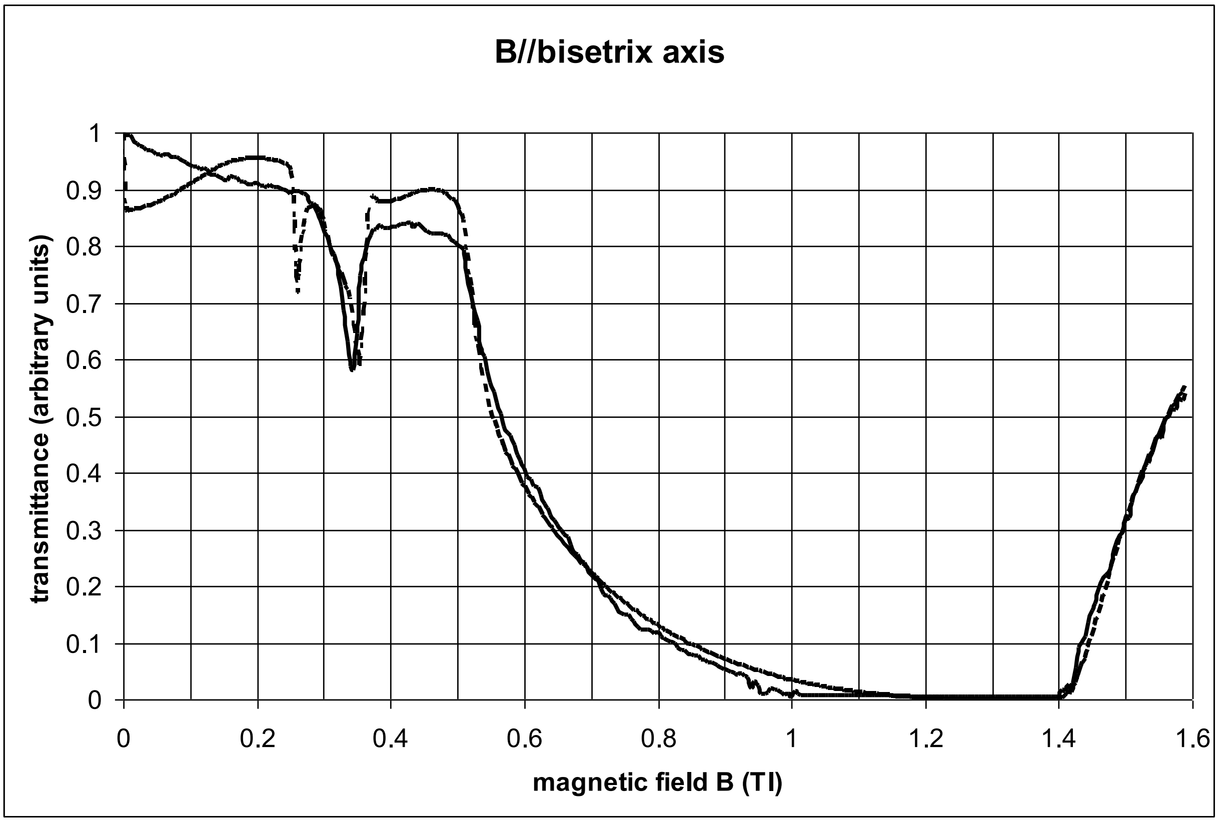


Fig. 12. Results of modeling of the form of line of the magnetooptical experiment when the magnetic field is oriented along bisectrix axis. Solid line is experimental results, dashed line – the best fitting.

We created this sharp maximum in the derivative of the real parts of a dielectric function for extraordinary Voigt wave by using the step function dependence of the charge density from magnetic field (fig. 11). The physical reason for this procedure is the following; at this magnetic field the contribution of holes is appeared in the magnetooptical response. The charge density of holes equals the charge density of electrons for bismuth. In modeling experiment the charge density after *B*=1.87 Tl is almost two times greater than before this magnetic field.

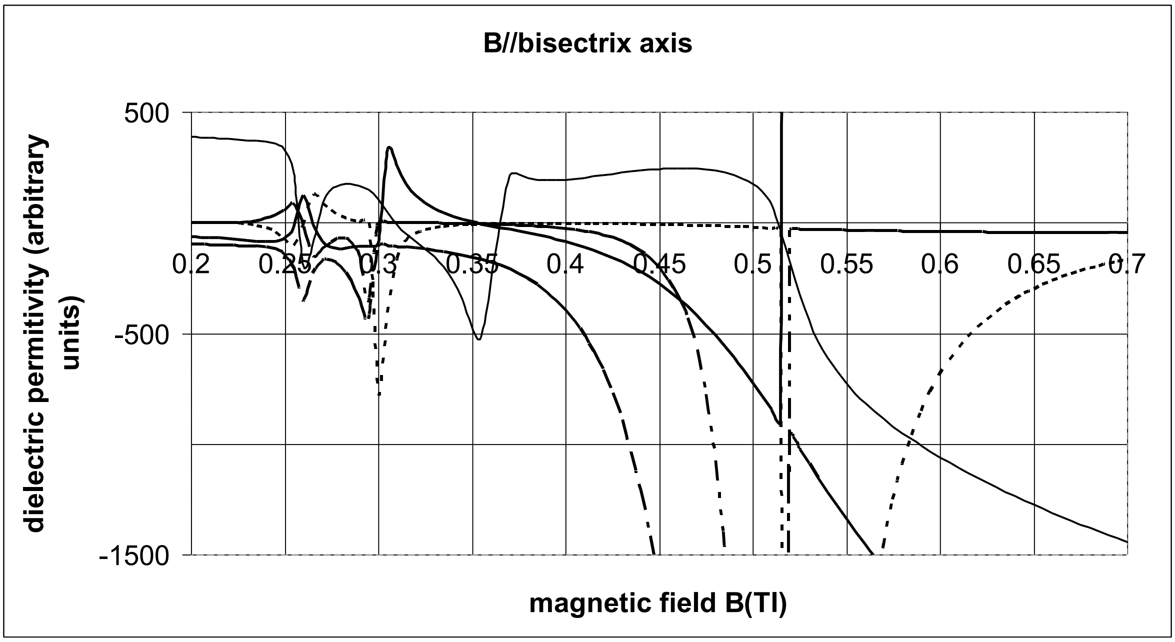


Fig. 13. Results of modeling of the form of line of the magnetooptical experiment when the magnetic field is oriented along bisectrix axis: real parts of a dielectric functions (solid line) for extraordinary and (dashed-point line) for ordinary, imagine parts (dashed lines) for extraordinary and (dashed-two-point line) for ordinary Voigt waves.

Numerical results when the magnetic field is oriented along bisectrix axis

The results of modeling (dashed line) of the form line of magnetooptical experiment (solid line) when the magnetic field is oriented along bisectrix axis are presented on the fig. 12 are presented. The physical situation in this orientation of the vector of magnetic induction relative crystallographic axis is the most complicated. There are three kinds of charge careers. These are the electrons with effective masses differed 2 times and heavy holes. The effective masses of the light bisectrix electrons are slightly less than the effective masses of the light binary electrons.

To analyze the structure of the magnetotransmittance we draw for the best fitting real (bold solid lines) and imagine (dashed lines) parts of a dielectric functions for ordinary (lower intensity) and extraordinary (greater intensity) Voigt waves (fig. 13). The absorption is started when real part of the dielectric function becomes positive and finished when real part of the dielectric function becomes negative.

We tried to separate signals from other kinds of charge carriers. With this aim we provided special numerical experiment. In components of the tensor of conductivity we successively canceled members for all charge extremums. Results of this experiment are submitted on the fig. 14.

We can see on fig 14 that when we are using only electrons for modeling form of line, there are not increasing the transmittance in the range magnetic field *B*≥1.4 Tl. Because this future is the result of equality to zero the real part of a dielectric function for extraordinary Voigt wave, this means, that it is response of holes in T-point of Brillouin zone. This point of view supported the behavior of the curve “bc” on the fig 14.

This dielectric function is calculated in assumption that there are only electrons of greater masses and holes.

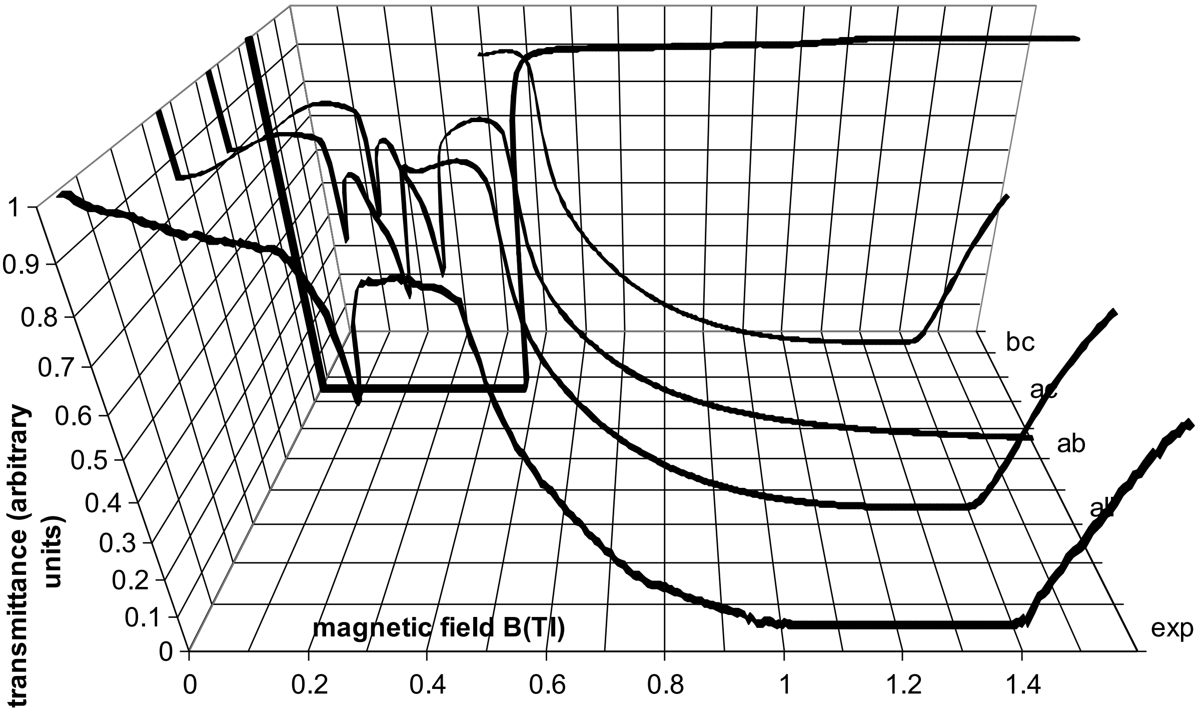


Fig. 14. Results of modeling of the form of line of the magnetooptical experiment when the magnetic field is oriented along bisectrix axis: exp - experimental result, all - the best fitting, ab – only electrons, ac – light bisectrix electrons and holes, bc - heavy bisectrix electrons and holes.

The mathematical picture becomes more clear after calculating the dielectric functions for each extremum. First we must tell that ordinary wave is not important for this direction of the magnetic field, because the corresponding dielectric function in all range of magnetic induction is less than zero. On the fig. 15 are represented results of modeling of dielectric function for all kinds of charge carriers and sum of them. This numerical calculation permit us to determine that singularity at B=0.25 Tl is cyclotron resonance of the light bisectrix electrons. It is wonderful, but at the experiment there is not this structure. Structure at *B*=0.35 Tl is appeared like result of complex combination of components of the high frequency conductivity tensor.

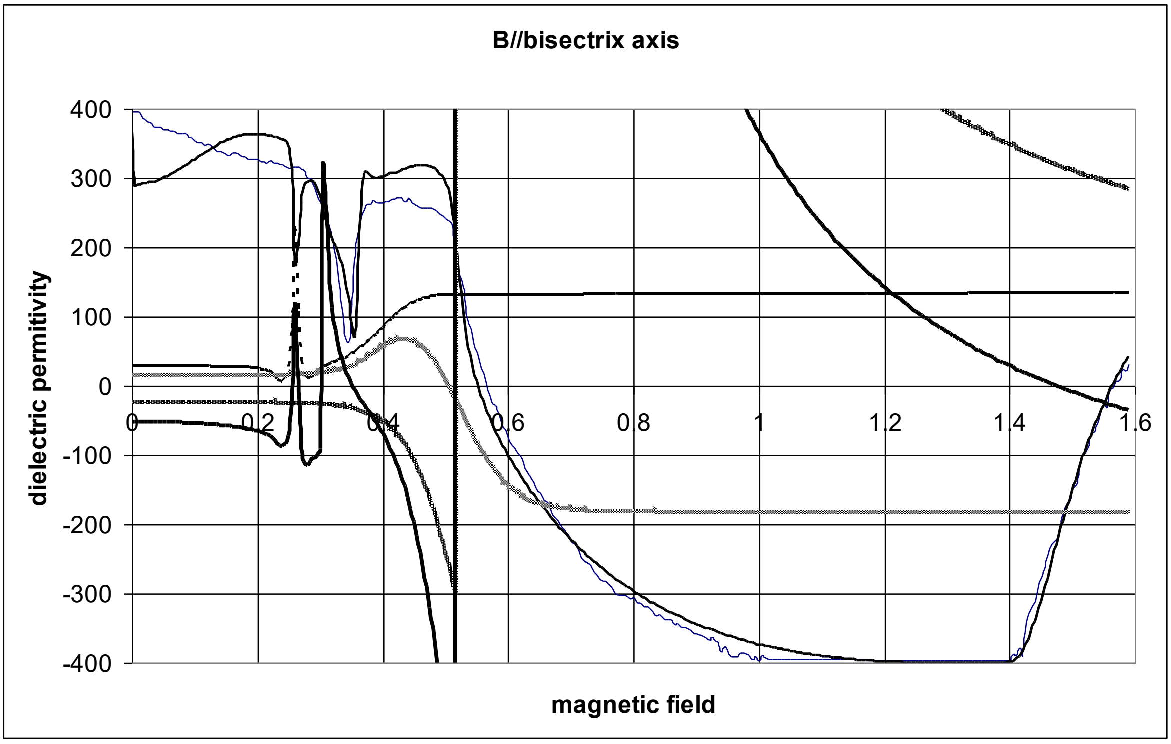


Fig. 15. Results of modeling of the form line of the magnetooptical experiment when the magnetic field is oriented along bisectrix axis: experimental curve (very thin solid line), the best fitting (thin solid line), real part of a dielectric functions (bold solid line) for extraordinary Voigt wave for calculation in framework of whole model, (dashed line) for calculation in framework of partial model (only light electrons), gray-black line – heavy electrons, gray line - holes.

SOLUTIONS AND RECOMMENDATIONS

The article was devoted to reproduce a magnetooptical experimental line with all details. Previous calculation [7] repeated form of the experimental line only qualitatively. We carried out a numerical experiment and remarked that some parameters needed a special consideration.

First we modeled the charge carrier density; it was found to be constant with one value for small magnetic field and other value for bigger magnetic field so there we needed to link both parts of behavior. The step functions were designed for that (Fig. 6 and 11). Second the lattice permittivity (Fig. 7) was modeled like step function and also the relaxation time. It is means that bismuth electronic and hole subsystems respond relatively independent on the action of the electromagnetic wave.

A deep analysis shows that not all electrons will participate in absorption of electromagnetic energy as we are using a spectrum in the far infrared range. Only approximately tenth of electrons in each ellipsoid will be excited (Fig. 5).

There is a wonderful result that we have got; when the magnetic field was oriented parallel the bisectrix direction, we observed in our calculations a cyclotron resonance around the magnetic field B = 0.25 Tl this feature does not exist in the experimental results (see the Fig. 12).

CONCLUSION - FUTURE RESEARCH DIRECTIONS

Attempts to calculate the permittivity of a planar waveguide for the sum over all electron and hole extremes of the valence and conduction bands of the high-frequency permittivity did not lead to acceptable results. In this approximation it was not possible to reconstruct the shape of the experimental magneto-optical spectrum with all the details. Therefore, the calculation of the permittivity of the planar waveguide was performed separately for each energy extremum. This may be for at least two reasons.

First, the bismuth monocrystal reacts to the external influence (electromagnetic wave) as several nested sublattices, weakly connected with each other. This is confirmed by the different values of the concentration of charge carriers concentrated at different points of the Brillouin zone, as well as by the corresponding relaxation times of the charge excitation and the lattice part of the permittivity.

Secondly, the peculiarity of the considered experiment is that the crystal is in a strong magnetic field, when Landau's magnetic quantization is essential. Moreover, for electrons with the smallest effective cyclotron masses in the bisector and binary directions, the ultraquantum limit of the magnetic field is reached. Therefore, a natural extension of this study is to simulate when the material properties of the waveguide walls would be taken into account by quantum mechanics methods, since under conditions of magnetic quantization the charge carriers are placed on Landau cylinders. Such formulation of the problem requires consideration of intraband transitions of electrons between Landau levels of conduction band at L Brillouin point, and holes in valence band at T Brillouin point.

The presented calculation model is implemented in a single program file. Taking into account quantum transitions of electrons, taking into account the selection rules for allowed optical transitions, the energy position of the Fermi level depending on the magnetic field, and the value of matrix elements of the velocity operator leads to the need for a modular organization of the algorithm for the numerical calculation of the permittivity of the planar waveguide.

CONCLUSION

Numerical calculation of the absorption of radiation, which has a pronounced resonance character, by the walls of a planar waveguide made of bismuth monocrystal placed in a magnetic field was performed. Such features of radiation transmission observed in the experiment were presumably associated with cyclotron absorption of the electromagnetic wave. Based on this assumption, the dependence of the transmission coefficient of the planar waveguide on the magnetic field value was calculated, which coincided with the experimental data in the orientation when the magnetic field vector is directed along the binary, bisector and trigonal axes of the bismuth crystal lattice. The experimentally observed magnetic absorption bands are formed by resonant cyclotron absorption of an electromagnetic wave propagating in a planar waveguide.

The absorption band with a minimum at B=0.35 Tl is formed by the cyclotron resonance of electrons of less effective mass at the L point of the Brillouin zone.

The absorption band in the range of magnetic fields $0.6 \le B \le 1.3$ Tl is formed by the cyclotron resonance of holes of the valence band at the T point of the Brillouin zone.

It is proved that in conditions of strong anisotropy of properties and the presence of topologically isolated Fermi surfaces the simulation of the experimental magneto-optical spectra is successful when the parameters of each extremum of the charge carriers are taken into account separately.

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