# Computer simulation of conoscopic patterns for gyrotropic birefringent crystals

Yu.A.Nastishin, O.G.Vlokh, O.B.Dovgyi

Institute of Physical Optics, 23 Dragomanov Str., Lviv 79005, Ukraine

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## Abstract

The algorithm for computer simulations of the conoscopic patterns for gyrotropic birefringent crystals is proposed. Traditional approach to the analysis of the conoscopic patterns is based on the approximations reducing the original phase retardation function to the equation of a circle, ellipse or hyperbola. Our computer simulations are based on the complete expressions describing the light propagation in a gyrotropic crystal without expansions of the complicated functions in a series. The simulated conoscopic patterns for one and two crystalline plates with symmetrically tilted optical axes (double-plate) are represented. The shape of the isochromes is discussed. The simulated patterns reproduce an experimentally observed phenomenon of the existence of circular isochromes at a non-zero tilt angle $\theta_c$ of the optical axes for the double-plate. The $\theta_c$ values deduced from the computer simulated patterns well agree with the values estimated from an approximate expression for $\theta_c$ earlier found in [Vlokh O.G., Kobylyanskyi V.B., Lazko L.A. Ukr. Fiz. Zhurn., N10, pp.1631-1638 (1974)].

**Keywords:** Optical conoscopy, gyrotropic birefringent crystals, computer simulation.

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## 1. Introduction

Conoscopy as an optical crystal characterization technique being quite simple in its experimental realization, in fact replaces many procedures which have to be performed to probe the light propagation in a crystal in different directions. Sending a diverged light beam on the crystal which is placed between crossed polarizers one obtains an interference pattern (conoscopic figure) usually composed of two sets of lines: isogyres and isochromes. Analyzing the conoscopic figure several important crystal characteristics (type of crystal (uniaxial or biaxial), optical sign, orientation of the optical axis (axes), presence and sign of gyrotropy, birefringence value) can be easily determined following the simple procedures well described in literature (see for example [1-4]). The analysis of the conoscopic pattern is based on the theory of light propagation in a crystal for different directions [2]. Although in principle the light propagation in crystals is well understood, the analysis of the conoscopic patterns is not always trivial. This especially concerns to the situations when a given conoscopic pattern results from the light interference in more than one crystal plate or when the crystal is distorted. In these complicated cases the isochrome and isogyre equations are of transcendental type and not always can be easily transformed to the equations of second order lines (circle, ellipse or hyperbola). As a matter of fact even in the simplest case of an uniform uniaxial crystal one has to use an approximation expanding complicated functions in a series. The approximation procedure is quite laborious and requires careful selecting of important terms according to their weights and proving the series truncation. In most practical cases the fine structure of the conoscopic pattern is lost after the simplifications.

Another way to analyze the complicated functions describing a conoscopic pattern is to generate their so-called Density Plot using advanced programming software as for example Mathematica or Maple [5]. These programming packages allow to work with exact expressions without approximations. The Density Plot package maps values of function $f(x,y)$ as points of different brightness such the value $f(x,y)=0$ is represented by a black dot in a given point $(x,y)$, the highest $f$ value corresponds to a white dot and the intermediate values are plotted as dots of corresponding gray levels. The Density Plot of the calculated light intensity function $I(x,y)$ for the conoscopic pattern looks one to one as corresponding experimental conoscopic figures. In our previous paper [5] we proposed an algorithm for computer simulation of conoscopic patterns for distorted uniaxial nematics. In this paper we extend this approach to the simulation of the conoscopic patterns for gyrotropic uniaxial crystals. We start with the plotting of conoscopic figures for a gyrotropic crystalline plate with tilted optical axes and then consider two gyrotropic crystalline plates with symmetrically tilted optical axes (further double-plate).

## 2. Algorithm for computer simulations of conoscopic patterns for gyrotropic birefringent crystals.

### 2.1. One gyrotropic crystalline plate.

The description of the conoscopic pattern for a gyrotropic birefringent crystal was performed for the first time in the paper [6]. The choice of the coordinate system in [6] was stipulated by the intent to simplify the isochrome equation. Here we work in the Cartesian coordinate system with its origin in the focus of the diverged beam. The focus of the diverged beam is located on the crystal first surface. The axis of the diverged light beam and the perpendicular to the crystal plate surfaces are oriented along $Z$-axis (Fig.1). The $X$-axis is chosen along the polarization direction of the first polarizer. The crystal is considered to be transparent. The orientation of the crystal optical axis is defined by the polar and azimuth angles $\theta$ and $\gamma$, respectively. The orientation of a given ray from the probing light beam is given by the polar and azimuth angles $\psi$ and $u$, respectively (Fig.2). In the calculations the second polarizer (analyzer) is considered to be in the immediate contact with the second crystal surface and serves as a screen. All optical elements are considered to be free of optical imperfections, and the efficiency of the polarizers to be independent on the polar angle of a light ray. The contributions of the reflection from the interfaces are neglected.

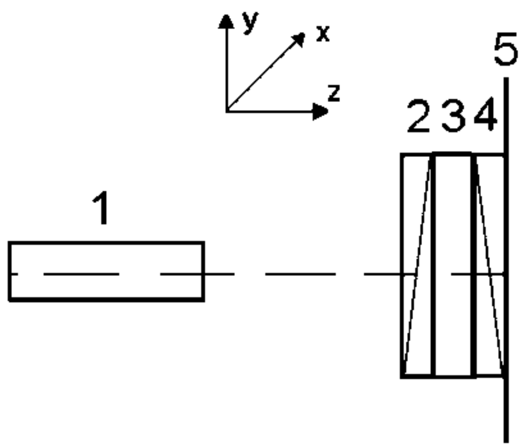



Fig.1. Cartesian coordinate system and experimental set-up; 1-laser, 2- polarizer, 3- crystal plate (plates), 4- analyzer, 5-screen.

The light intensity passed through the crystal placed between the crossed polarizers (Fig.1) can be calculated using the Jonnes matrix formalism. The Jonnes matrix of a gyrotropic crystal with a desired azimuth orientation of the optical axis with respect to the light beam can be determined as:

$$
\begin{aligned}
&T_{11} = cos(\Delta/2) - \\
&- i\,[(1-k^2)/(1+k^2)]\, sin(\Delta/2)\, cos(2\chi), \\
&T_{12} = -T_{21} = -[\{2k/(1+k^2)\}+ \\
&+ i\,[(1-k^2)/(1+k^2)]\, sin(2\chi)]\, sin(\Delta/2), \\
&T_{22} = cos(\Delta/2) + \\
&+ i\,[(1-k^2)/(1+k^2)]\, sin(\Delta/2)\, cos(2\chi),
\end{aligned}
\qquad (1)
$$

where $\Delta$ is the phase retardation caused by the ***elliptical*** birefringence, k is the ellipticity of the eigenwaves in the crystal, $\chi$ is the azimuth angle of the principal plane (a plane containing the optical axis and the wave vector of a given light ray).

For one crystal plate placed between crossed polarizers the transmittance (intensity normalized by its value on the crystal's first surface) is of the form:

$$I = (Re[T_{12}])^2 + (\,Im[T_{12}])^2$$

and can be rewritten as:

$$I = \frac{[4k^2 + (1-k^2)^2 * sin^2(\Delta/2) sin^2(2\chi)]}{(1+k^2)^2} \qquad (2)$$

The elliptical phase retardation can be calculated as a geometrical average of contributions from linear and circular birefringence

$$\Delta = (2\pi n \Delta n/\lambda)* \\ (sin^4\phi + \{\eta_{//} cos^2\phi + \eta_{\perp} sin^2\phi\}^2)^{1/2}, \qquad (3)$$

where $n$ is the average refraction index, $\Delta n = n_{//} - n_{\perp}$ is the difference between the refractive indices along and perpendicular to the optical axis, respectively, $\eta_{//} = 2g_{//}/(n\,\Delta n)$, $\eta_{\perp} = 2g_{\perp}/(n\,\Delta n)$, $g_{//}$ and $g_{\perp}$ are the gyration parameters along and perpendicular to the optical axis, $\phi$ is the angle between the optical axis and the wave vector of a given light ray. The expression defining the angles $\phi$ and $\chi$ in

$$cos\phi = [d\,cos\theta + sin\theta\,(x\,cos\gamma + y\,sin\gamma)]/(x^2+y^2+d^2)^{1/2}, \qquad (4)$$

$$cos\,\chi = \frac{(x\,cos\theta - d\,sin\theta\,cos\gamma)}{[(x\,cos\theta - d\,sin\theta\,cos\gamma)^2 + (y\,cos\theta - d\,sin\theta\,cos\gamma)^2]^{1/2}}, \qquad (5a)$$

$$sin\gamma = \frac{(y\,cos\theta - d\,sin\theta\,cos\gamma)}{[(x\,cos\theta - d\,sin\theta\,cos\gamma)^2 + (y\,cos\theta - d\,sin\theta\,cos\gamma)^2]^{1/2}}. \qquad (5b)$$

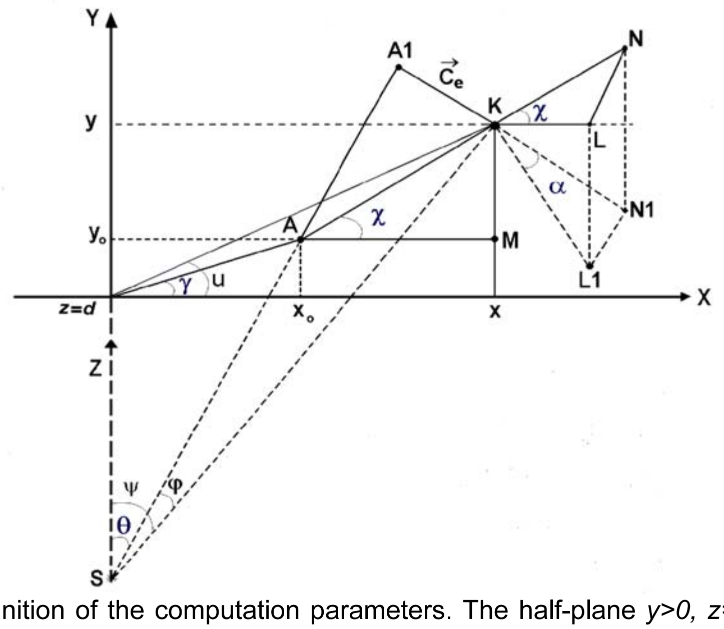



Fig.2. To the definition of the computation parameters. The half-plane *y>0, z=d* is in the plane of the page and is overlapped with the analyzer and screen planes. For the convenience the half-plane *y=0, 0<z<d* is depicted in the plane of the page but keeping in mind that really this plane is perpendicular to the half-plane *y>0, z=d*. *S* is the origin of the coordinate system. *A* and *K* are located in the plane *z=d* and are the exit points of the optical axis *SA* and of a given ray *SK* with the wave vector ***k***, of the diverged light beam, respectively. *K(x,y)* is a given point of the conoscopic pattern

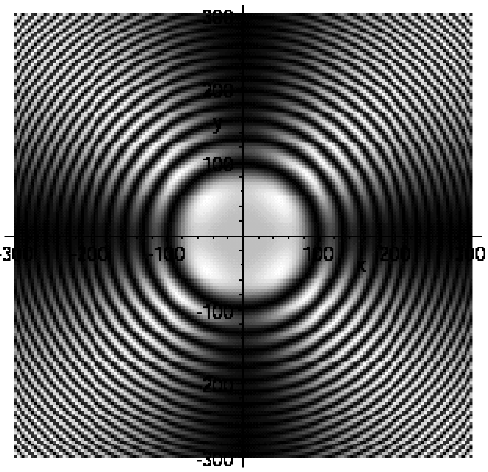
Cartesian coordinates are in the form [5]

Following [2,3] the ellipticity $k$ of the eigenwaves can be written as

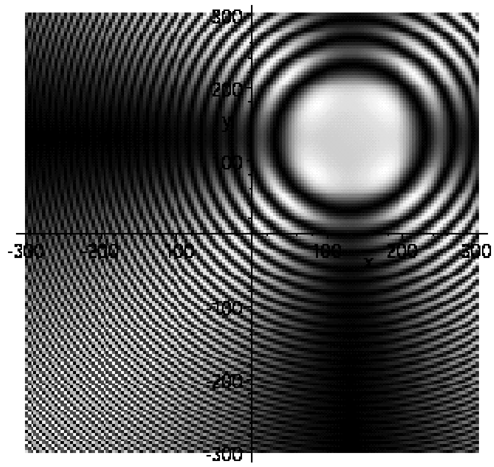
$$k=\frac{sin^2\phi-\sqrt{sin^4\phi+\{\eta_{//}\cos^2\phi-\eta_{\perp}\sin^2\phi\}^2}}{\{\eta_{//}\cos^2\phi-\eta_{\perp}\sin^2\phi\}^2} \qquad (6)$$

The system of equations (2-6) is the algorithm for generating the Density Plot of the function $I(x,y)$. The simulated conoscopic patterns for different angles $\theta$ with some typical crystal parameters are shown in Fig.3. It is seen that for $\theta=0^o$ the isochromes are circles centered on the axis of the light beam as it is for a non-gyrotropic birefringent crystal. Indeed, for $\psi=const$ substituting (3) in (2) we obtain the equation of a circle with the radius $\Delta$, namely $(\partial\Delta/\partial u)=0$ at $\theta=0$. However in contrast to the conoscopic pattern for a non-gyrotropic crystal the isogyres disappear before they approach the center. Because of the non-zero $g_{//}$ the center of the conoscopic figure might be dark (when $\Delta=2\pi m$, m is an integer number) or bright ($\Delta\neq 2\pi m$).

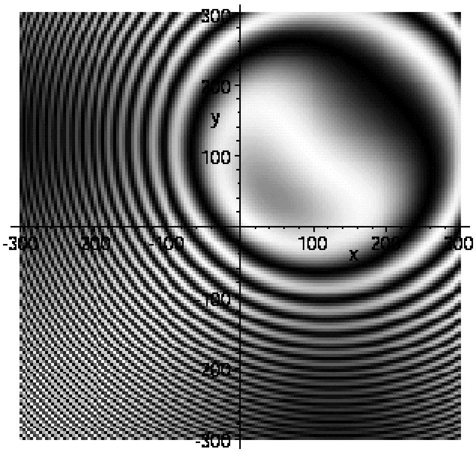
When $\theta>0$ the isochromes are not circular. They are self-closed curves at $0<\theta<.54.5^o$ (further small $\theta$) and broken ones at $54.5^o<\theta<.90^o$ (further large $\theta$). In the first approximation these curves can be modelled by an ellipse or hyperbola at small and large $\theta$, respectively. Our analysis shows that for the gyrotropic crystals at



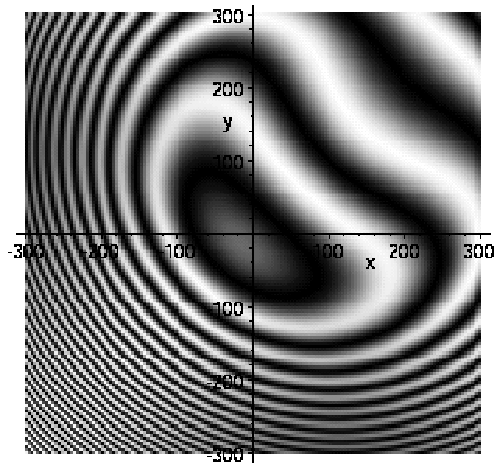
a) $\theta=0^0, g_u=0.0005$



b) $\theta=13^0, g_u=0.0005$



c) $\theta=13^0, g_u=0.005$



d) $\theta=13^0, g_u=0.01$

Fig.3. Computed conoscopic patterns for a single gyrotropic crystalline plate with $\Delta n=0.1$, $g_{xx}=0$. The isochromes are circles centered on the axis of the probing light beam at $\theta=0^o$ – *a)*. At nonzero $\theta$, for example $\theta=13^o$ the isochromes are self-closed curves of a complicated shape different from the shape of an ellipse when the parameter $\eta=2g_{zz}/\Delta n$ increases: $g_{zz}=0.0005$ – *b*, $g_{zz}=0.005$ – *c*, $g_{zz}=0.01$ – *d*.

small $\theta$ the isochromes shape essentially differs from the shape of an ellipse when $g_{//}$ is large (see Fig. 3c,d). The isochromes are rather of the bean type contour than simply elliptical. They are concave out from center and convex in the direction to the center. The concavity-convexity of the isochromes is small for typical crystal values. However it becomes well visible for large $g_{//}$ in the computer simulations (Fig.3d). One has to notice that the isochrome shape is defined by the parameter $\eta = 2g_{zz} / \Delta n$ (here we take $g_{xx}=0$). Hence, $\eta$ can be large when $\Delta n$ is small. The situation of small $\Delta n$ can be realized near the isotropic point [7]. We are considering this situation in our forthcoming paper.

One more difference between the conoscopic patterns for non-gyrotropic and gyrotropic crystals was documented in the paper [6]. It was shown experimentally that for two gyrotropic crystal plates with symmetrically tilted optical axes at $\theta$ increasing, the shape of the isochromes becomes circular twice: at $\theta=0^o$ and at some special $\theta_c$ value, which depends on the $\eta$ parameter. As it was stated in [6] this effect exists also for one plate. The action of the second plate is to produce additional isochromes centered around the center of the probed light beam. These new central isochromes also become circular twice in the same way as the isochromes centered around the exit points of the optical axes. In [6] the effect was analyzed analytically using several expansions of $\Delta$ in a series. The final expansion was truncated at the second order and the authors [6] have found an analytical expression for $\theta_c$:

$$sin^3\theta_c \approx 2^{1/2}\eta \qquad (7)$$

For a typical gyrotropic crystal $\eta$ takes a value from the range $10^{-2}\div10^{-3}$. Hence, according to [6], $\theta$ supposes to be a value between $7^o$ and $14^o$. Computer simulations based on the algorithm that does not involve any simplification expansions (see below) really reproduce isochromes transformations mentioned above. The values $\theta_c$ for which the isochromes become circular well agree with the expression obtained in [6]. The circular shape of the isochromes for typical $\eta$ values was really obtained at $\theta$ being between $7^o$ and $14^o$. The conoscopic pattern for two plates will be discussed below. Here we only point out that the circular isochromes also appear for one plate at $\theta=\theta_c$. The existence of

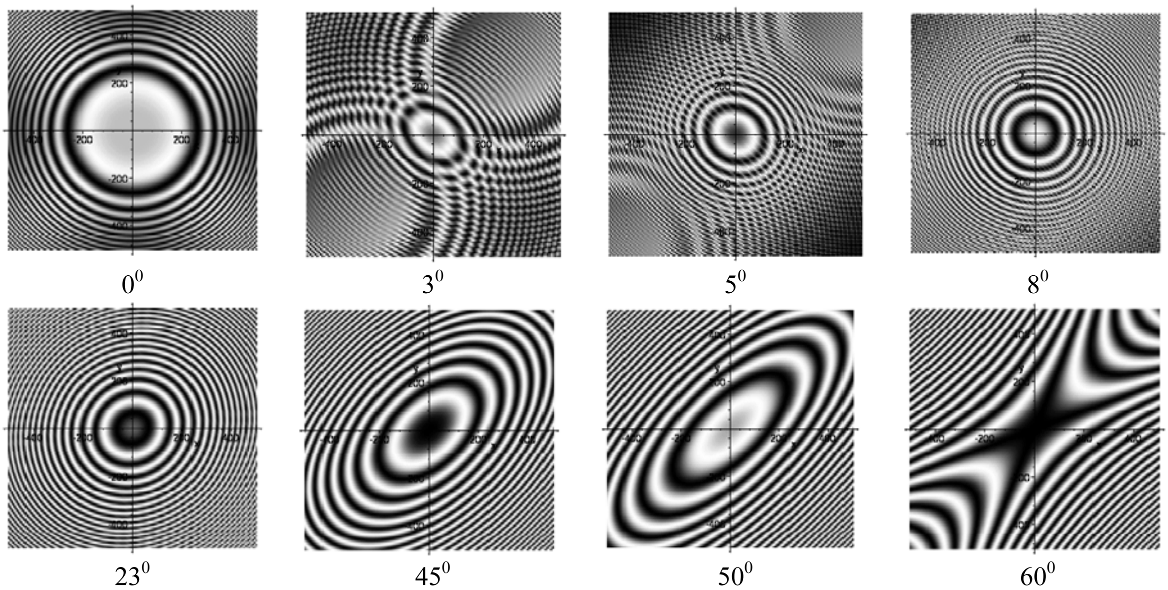



Fig.4. Computed conoscopic patterns for double-plate at different tilt angles of the optical axes.

the circular isochromes implies that for $\psi=const$

$$(\partial\Delta/\partial u)=0 \qquad (8)$$

at $\theta=\theta_c$. However substituting (3) directly in (8) we find that for all $\theta\neq0$ the left part of the equation (8) contains the terms depending on $u$ and $\psi$. Therefore for $\theta\neq0$ the isochromes never become true circles. Thus, the experimentally observed circular isochromes are circular only apparently. As it was mentioned above at $\theta\neq0$ the real isochromes are not exactly elliptical and as a result they are not ideal circles at $\theta=\theta_c$. Performing the expansions of $\Delta$ in a series one can approximate the real isochrome shape by an ellipse and then one can find $\theta_c$ at which the ellipse transforms into a circle. It follows from the experiment as well as from the computer simulations that the deviation from the circular shape is really small indicating that the mentioned approximation is valid.

## 2.2. Two gyrotropic crystal plates.

As mentioned above to find the transmittance of the light passed through two plates placed between the crossed polarizers we use the Jonnes matrix formalism. Finally we have:

$$I = (Re[T^{ab}])^2 + (Im[T^{ab}])^2,$$

where

$$T^{ab}=T^b_{11}\,T^a_{12} + T^b_{12}\,T^a_{22}\,, \qquad (9)$$

the indices $a$ and $b$ correspond to the orientations of the optical axes in the plates $a$ and $b$, so that the components of the matrix $T_{ij}$ given by the equations (1) have to be calculated with γ=45° for $a$ and γ=225° for $b$ plate. Substituting relations (1) in eq. 9 we have :

The light transmittance is of the form:

$$\begin{aligned} I=\;&c_1\sin^2[(\Delta_a+\Delta_b)/2]+\\ &2\{c_2\sin([\Delta_a/2])+c_3\sin([\Delta_b/2)\}*\\ &*\sin([\Delta_b/2)\sin[(\Delta_a+\Delta_b)/2]+\\ &c_4\sin^2(\Delta_a/2)\sin^2(\Delta_b/2)+\\ &c_5\cos(\Delta_a/2)\sin(\Delta_a/2)\sin^2(\Delta_b/2)+\\ &c_6\cos^2(\Delta_a/2)\sin^2(\Delta_b/2), \end{aligned} \qquad (10)$$

with

$$\begin{aligned} &c_1=s_1^2+s_4^2, \quad c_2=s_1s_3+s_4s_6,\\ &c_3=s_1s_2+s_4s_5,\; c_4=s_3^2+s_4^2,\\ &c_5=s_5s_6+s_2s_3,\; c_6=s_2^2+s_5^2, \end{aligned} \qquad (11)$$

$\Delta_a$, $\Delta_b$ $\sin(2\chi_a)$, $\cos(2\chi_a)$, $\cos(2\chi_b)$, $k_a$, $k_b$ can be calculated from equations (5a), (5b) and (6) substituting γ=45° for $a$ and γ=225° for $b$ plate.

The equation (10) together with notations for the coefficients is the algorithm for the calculation of the conoscopic pattern for the double-plate. Fig.4 shows the transformation of the double-plate conoscopic pattern at the $\theta$ increasing. We really find that the isochromes are circular twice: at $\theta=0$ and $\theta_c$, which for $\Delta n$=0.1 and $g_{//}$ =0.00025 appear to be about 9°. For the same values $\Delta n$ and $g_{//}$ the equation (7) gives $\theta$=8.76°. The agreement of the result obtained from the computer simulations and estimated from the theory [6] that involves the approximations confirms the validity of the approximations used in [6].

Simulated conoscopic patterns display the presence of a fine structure. Such a fine structure really was observed experimentally (Fig. 5) [3]. It is evident that this fine structure results from overlapping of the conoscopic pattern produced by each of the plates separately.

$$\begin{aligned} T^{ab}=\;&s_1\sin[(\Delta_a+\Delta_b)/2]+s_2\sin(\Delta_a/2)\cos(\Delta_b/2)+s_3\sin(\Delta_a/2)\sin(\Delta_b/2)+\\ &i\{s_4\sin[(\Delta_a+\Delta_b)/2]+s_5\sin(\Delta_b/2)\cos(\Delta_a/2)+s_6\sin(\Delta_a/2)\sin(\Delta_b/2)\} \end{aligned} \qquad (9a)$$

$$\begin{aligned} &s_1=-2k_a/(1+k_a^2), \qquad s_2=2(k_a-k_b)(1-k_ak_b)/(1+k_a^2)(1+k_b^2),\\ &s_3=(1-k_a^2)(1-k_b^2)\sin(2\chi_a)/(1+k_a^2)(1+k_b^2), \qquad s_4=(1-k_a^2)\sin(2\chi_a)/(1+k_a^2),\\ &s_5=2(k_a^2-k_b^2)\sin(2\chi_a)/(1+k_a^2)(1+k_b^2),\\ &s_6=\{k_a(1-k_b^2)\cos(2\chi_a)-k_b(1-k_a^2)\cos(2\chi_b)\}/(1+k_a^2)(1+k_b^2). \end{aligned} \qquad (9b)$$

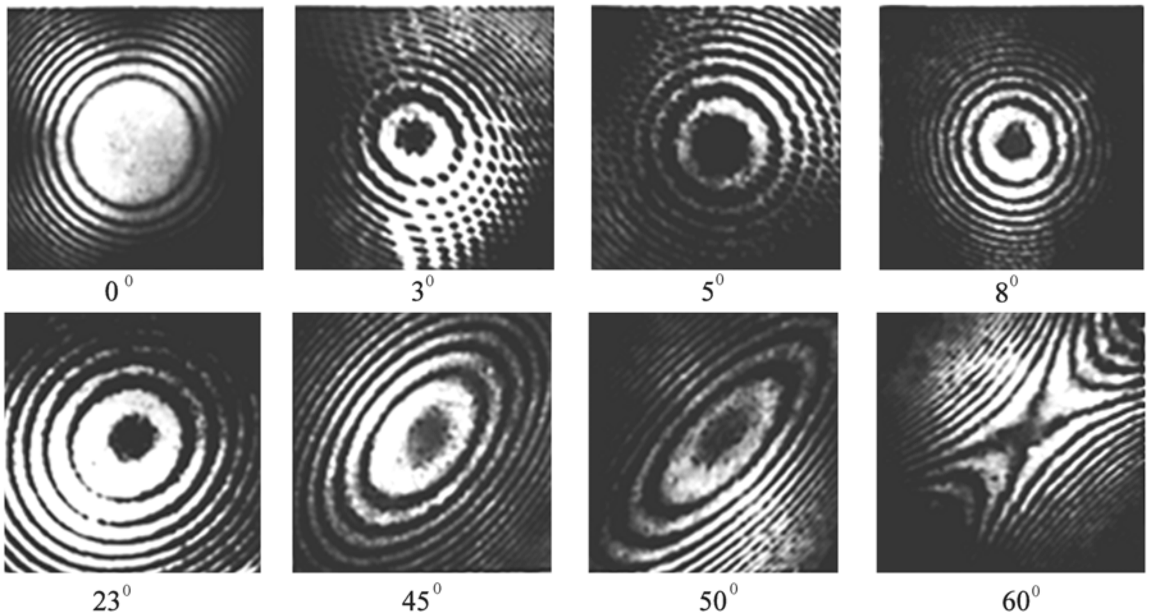



Fig.5. Experimental conoscopic patterns for double-plate of the crystal $LiJO_3$ at different tilt angles of the optical axes adopted from [3].

Zeroing the terms in (10) one can establish the contribution and role of each term in the transmittance expression. Computer simulations confirm that the isochromes centered on the axis of the light beam are described by the first term in eq. (10) as it was fairly stated in [6]. Solving the equation

$$(\partial(\Delta_a+\Delta_b)/\partial u)=0 \qquad (12)$$

together with the condition $\psi=const$ we obtain in the left part of eq. (12) a rigorous but quite long expression which contains the terms depending on $u$ as well as on $\psi$ . We do not represent this expression here. The presence of $u$- and $\psi$-depending terms implies that the isochromes centered on the axis of the light beam appearing to be circular at $\theta=\theta_c$ in fact exhibit a complicated fine structure. All terms in eq. (12) depending on $u$ have the coefficients proportional to $(\sin\psi\sin\theta)^m$ with $m$ being an integer number between 1 and 8. Neglecting these terms, omitting the terms with the powers of $\eta$ higher than 2 and vanishing $\psi$ we actually reduce the equation (12) to the equation of a circle and finally obtain it in a form

$$\sin^8\theta_c-\eta^2\sin^2\theta_c\,(2-3\sin^2\theta_c)=0 \qquad (13)$$

which for small $\theta$ takes the form (7) obtained for the first time in [6]. Therefore starting from the equations (12), substituting the phase retardations in the form given by equations (3) and (4) we came to the same result which was obtained in [6] by the expansion of the phase retardation function in a series.

## Conclusion

In this paper we have proposed an alternative approach to the analysis of the conoscopic patterns for gyrotropic crystals via computer simulations. In the computer simulations the conoscopic pattern is plotted using complete expressions describing the light propagation in the crystal, while the traditional analysis procedure requires approximate reducing of the original equation for the phase retardation to an equation of the second order curves. The simulated conoscopic patterns contain all the details of the experimentally observed conoscopic figures including their fine structure, and demonstrate the validity of the proposed algorithm. Computer simulations have also confirmed the algorithmic reliability of the traditional conoscopic analysis procedure.

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