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REFRACTOMETRY OF UNIAXIALLY COMPRESSED Rb₂SO₄ CRYSTALS

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ABSTRACT

Introduction. The refractive index n of a crystal is its fundamental characteristic. In the presence of the experimentally obtained dispersion $n(\lambda)$ with high accuracy, it is possible to determine the fundamental characteristics of single crystals using analytical relations for the refractive index in the region of crystal transparency.

Materials and Methods. In this work, high-optical-quality rubidium sulfate (Rb₂SO₄) single crystals were synthesized, crystallographic orientation was determined using a polarization microscope and conoscopic figures, and the dispersion of the refractive indices $n_x(\lambda)$ was studied using the Obreimov immersion method at room temperature for different directions of uniaxial compression with stress magnitude of $\sigma_m \sim 100$ bar.

Results and Discussion. It was found that the refractive indices dispersion of this crystal $n_i(\lambda)$ is normal ($\partial n / \partial \lambda < 0$). As the fundamental absorption edge is approached, it increases sharply for the three polarization directions of the electromagnetic wave. The refractive indices satisfy the inequalities $n_x \geq n_z > n_y$ and $dn_x/d\lambda > dn_z/d\lambda > dn_y/d\lambda$.

The baric changes in the molar refraction R_i , electronic polarizability α (for the wavelength $\lambda = 500$ nm), and crystal-optical parameters (spectral positions of the effective centers of ultraviolet and infrared oscillators, as well as their effective strengths) of Rb₂SO₄ crystals at room temperature were calculated. It was found that uniaxial pressures of $\sigma \sim 100$ bar led to an increase in electronic polarizability of the crystal by an average of $(1 - 3) \times 10^{-26} \text{ cm}^3$.

Conclusion. It was established that uniaxial pressures lead to an increase in contributions from infrared oscillators by 2–5 %, primarily due to the baric dependence of the optical isotropic point. They also shift the position of the effective strength of the ultraviolet oscillator λ_{0i} toward the short-wavelength region of the spectrum. The change in the effective oscillator strength in this baric range does not exceed 1 %. It was found that the positions of effective absorption bands are more sensitive to uniaxial pressures than the effective strengths of the corresponding oscillators.

Keywords: refractive indices, uniaxial compression, refraction, electronic polarizability, band gap width.

INTRODUCTION

The refractive index (RI) n of a crystal, which is determined by its electronic subsystem for a certain photon energy $\hbar\omega$ or wavelength λ , is its fundamental characteristic. The spectral dependence of the refractive index $n(\lambda)$ in a wide spectral region of the material's transparency contains significantly more information about its optical-electronic parameters.



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The most accurate RI is determined for transparent materials in the visible and near ultraviolet (UV) and infrared (IR) regions of the spectrum with an error of the order of $\pm 2 \times 10^{-5}$, but in several individual cases it can be $\pm 5 \times 10^{-6}$ [1-8]. Transparent materials in the specified regions of the spectrum include dielectrics and semiconductors with average bandgap widths ($E_g \sim 4 \dots 6$ eV). In the presence of the experimentally obtained dispersion $n(\lambda)$ with high accuracy, it is possible to determine the fundamental characteristics using analytical relations for the RI in the region of crystal transparency.

To describe the dependence of $n(\lambda)$, theoretical models of the atomic structure of the crystal are used, in which there is a dependence of the polarization of the medium on the frequency of the electromagnetic wave. If attenuation, nonlinearity, and spatial dispersion are neglected, then we can assume that the electrons behave similarly to the influence of the quasi-elastic force $\mathbf{F} = -q\mathbf{r}$ on their deviation from the equilibrium position:

$$r = \frac{eE}{m(\omega_0^2 - \omega^2)}, \quad (1)$$

where ω is the cyclic frequency of the electromagnetic wave $\mathbf{E} = \mathbf{E}_0 \exp(-i\omega t)$, $\omega_0 = \sqrt{q/m}$ – the resonant frequency.

Each electron creates a dipole moment $\mathbf{p} = e\mathbf{r}$. The nuclei also contribute to the polarization of the crystal, but since their mass is large compared to the mass of the electron, their contribution in the first approximation can be neglected. The frequency dependence of RI is as follows:

$$\frac{n^2 - 1}{n^2 + 2} = \frac{4\pi}{3} N \frac{e^2}{m} \sum_k \frac{f_k}{\omega_k^2 - \omega^2}, \quad (2)$$

where N is the number of electrons for the corresponding resonant frequency ω_k , f_k is the oscillator strength, which determines the degree of electron participation in this oscillation.

If in relation (2) we consider only two oscillators in the near UV and IR regions of the spectrum, then we can obtain the well-known Selmeyer formula:

$$n_i^2 = 1 + \frac{B_1 \lambda_{01}^2 \lambda^2}{\lambda^2 - \lambda_{01}^2} + \frac{B_2 \lambda_{02}^2 \lambda^2}{\lambda_{02}^2 - \lambda^2}. \quad (3)$$

Here λ_{01} and λ_{02} are the spectral positions of the effective centers of the UV and IR oscillator bands, respectively, and B_1 and B_2 are the effective strengths of the corresponding oscillators.

The study of baric changes in the RI is due to the study of existing or possible phase transitions, as well as changes in the structure during temperature changes or compression of the crystal. Baric dependences of the RI have recently been actively studied, although the emphasis is on the influence of hydrostatic pressure [9 – 16].

It has been found that the RIs decrease on average by 4 % in the pressure range up to 15 kbar [5, 6] for several crystals that are actively used in multiplet quantum laser sources (InGaAsP, AlGaInAs, and GaInNAs). For sapphire crystals at pressures up to 190 kbar, the refractive index at a light wavelength of 514.5 nm decreases linearly [11]. For KMgF_3 crystals, the refractive index increases monotonically under pressure: $dn/dp = 2.46 \times 10^{-4} \text{ bar}^{-1}$ for $\lambda = 589.3$ nm [12]. In some crystalline dielectrics, it has been found that the RIs mostly increase during uniaxial compression [13 – 16].

This behavior of RI is caused by the fact that hydrostatic pressure reduces the volume of the crystal and increases its density, which causes the growth of RI. The effect of uniaxial pressure on the refractive properties of crystals can be similar. At the same time, in anisotropic crystals, uniaxial compression along a certain direction will not always lead to unambiguous changes in the volume and RI in other crystallo-physical directions. Therefore, it is interesting to evaluate the effect of uniaxial compression on the RI of anisotropic crystals.

MATERIALS AND METHODS

We consider the effect of uniaxial compression σ_m on the behavior of the RI of a rubidium sulfate (RS) Rb_2SO_4 crystal. This is a typical representative of the ABSO_4 group crystals; at a temperature of $T_c \sim 922$ K, it undergoes a phase transition from the pseudohexagonal paraelectric phase $P-3m1$ to the orthorhombic ferro-elastic phase (symmetry space group $D_{2h}^{16} - Pmcn$) [17, 18]. The study of their crystal structure allowed us to clarify the lattice parameters: $a = 7.82079(10)$ Å, $b = 5.97778(7)$ Å, and $c = 10.44040(13)$ Å, and the band-energy structure of the crystal has a direct-type band gap ($E_g = 4.89$ eV) and weak dispersion of energy levels. It was also established that for this crystal, the top of the valence band is formed by $2p$ states of oxygen atoms, and the bottom of the conduction band is formed by $4s$ -electrons of rubidium [17, 18].

Previously, an optical isotropic point (OIP) was found in this crystal at room temperature: the equality of n_z and n_y at a wavelength of $\lambda = 495$ nm and room temperature ($n_z = n_y = 1.51705$) [19-21]. The study of the dispersion dependences of birefringence $\Delta n_i(\lambda)$ showed that the crystal has a small normal dispersion $d(\Delta n_x)/d\lambda \leq 0$, and uniaxial compressions σ_m do not change the character, but only the magnitude of the slope of the curves $\Delta n_i(\lambda)$ [22]. The authors also calculated the spectral dependences of the combined piezocoefficients $\pi_{im}^0(\lambda)$ and found that they are piezocoefficients π_{31}^0 and π_{21}^0 in the vicinity of the OIP at a wavelength of $\lambda = 490$ nm are equal.

The analysis of baric changes in the main RIs $n_i(\sigma_m)$ of the RS crystal was carried out based on previously obtained dependencies $\pi_{im}^0(\lambda)$ using the formula:

$$n_i(\lambda, T) = n_{i0}(\lambda, T) - \frac{1}{2} \pi_{im}^0(\lambda, T) \sigma_m n_{i0}^3(\lambda, T), \quad (4)$$

where n_{i0} is the refractive index of a mechanically free crystal,
 σ_m is the magnitude of the mechanical load applied to the crystal,
 π_{im}^0 are the absolute piezo-optical constants,
index i denotes the direction of light,
index m denotes the direction of compression.

This research method allows us to study the behavior of all the main RIs under the action of pressures in a wide spectral region along different crystallographic directions (especially the behavior of n_i under the action of σ_i). The baric behavior of RIs n_i ($i \neq m$) can be directly investigated by the well-known direct interference-optical method [2, 3], but only for one wavelength, and it is experimentally more complicated.

RESULTS AND DISCUSSION

Fig. 1 shows the dispersion dependences of n_x at room temperature of mechanically free and uniaxially compressed RS crystals. In general, it was established that the dispersion of the RI $n_i(\lambda)$ of this crystal is normal ($\partial n / \partial \lambda < 0$), and increases rapidly with the approach to the edge of fundamental absorption, $n_i(\lambda)$ for three directions of

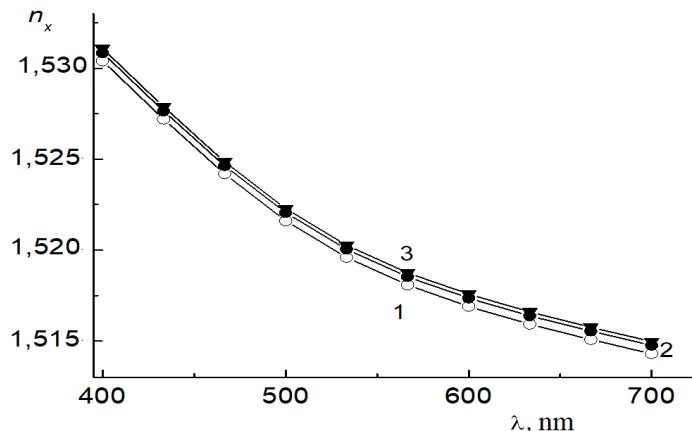


Fig. 1. Dispersion of refractive indices $n_x(\lambda)$ of Rb_2SO_4 crystals for different directions of uniaxial compression: 1 – $\sigma_m = 0$, 2 – $\sigma_z = 100$ bar, 3 – $\sigma_y = 100$ bar.

polarization of the electromagnetic wave. The following relations between the RI were found: $n_x \geq n_z > n_y$ and $dn_x/d\lambda > dn_z/d\lambda > dn_y/d\lambda$. It was established that the uniaxial pressure does not change the character of the curves $n_i(\lambda)$, only the value of the dispersion $dn_i/d\lambda$ changes. Table 1 shows the corresponding values for all crystallographic directions under the action of different pressures.

Let us consider the relationship $n_i(\lambda, \sigma)$ with the characteristics of the crystal, which follow from the dispersion formula of Selmeyer and the Lorentz-Lorentz formula, which describes refraction and electronic polarizability [1, 2]:

$$\alpha = \frac{3}{4\pi N} \frac{n^2 - 1}{n^2 + 2} \quad (5)$$

Table 1. Baric changes in the specific refraction R_i and electronic polarizability α_i for the light wavelength $\lambda = 500$ nm, as well as the crystal-optical parameters of Rb_2SO_4 crystals at a temperature of $T = 293$ K

Parameters	$\sigma_m = 0$ bar	$\sigma_x = 100$ bar	$\sigma_y = 100$ bar	$\sigma_z = 100$ bar
$\alpha_x \times 10^{24}$, cm^3	8.85	8.87	8.88	8.88
$\alpha_y \times 10^{24}$, cm^3	8.83	8.85	8.85	8.86
$\alpha_z \times 10^{24}$, cm^3	8.84	8.86	8.87	8.86
R_x , cm^3	22.34	22.37	22.36	22.35
R_y , cm^3	22.30	22.31	22.32	22.33
R_z , cm^3	22.31	22.34	22.33	22.33
λ_{0x} , nm	94.19	94.25	94.23	94.23
λ_{0y} , nm	93.41	93.43	93.45	93.46
λ_{0z} , nm	94.18	94.19	94.21	94.22
$B_x \times 10^6$, nm^{-2}	141.15	141.13	141.12	141.12
$B_y \times 10^6$, nm^{-2}	143.83	143.81	143.82	143.80
$B_z \times 10^6$, nm^{-2}	141.16	141.13	141.14	141.12

$$R = \frac{4\pi}{3} N_A \alpha = \frac{\mu n^2 - 1}{\rho n^2 + 2}. \quad (6)$$

Here N is the number of particles per unit volume; N_A is Avogadro's number; μ is the molar mass; ρ is the density of the crystal.

Using the obtained dependences $n_i(\lambda, \sigma)$, according to formulas (3), (5) and (6), the parameters listed in Table 1 were calculated. The calculated refractions of the RS crystals agree well with the sum of the individual refractions of the structural elements

$$R(\text{Rb}_2\text{SO}_4) = 2R(\text{Rb}) + R(\text{SO}_4) = 10 + 14.5 = 24.5 \text{ cm}^3/\text{mol}. \quad (7)$$

This suggests that Rb^+ cations make a significant contribution (~ 41 %) to the total refraction of the studied crystals. If we compare the crystal-optical parameters of these crystals with isomorphic $(\text{NH}_4)_2\text{SO}_4$, LiNH_4SO_4 , K_2SO_4 and RbNH_4SO_4 , we can see that the cationic substitution $\text{Li}^+ \rightarrow \text{Rb}^+$ causes an increase in the RI on average by $3-5 \times 10^{-3}$, shifts the position of λ_{0x} by approximately 7 nm towards the short-wavelength, and the position of λ_{0z} – by 3 nm towards the long-wavelength parts of the spectrum. In general, it was established that the substitution $\text{Li}^+ \rightarrow \text{K}^+ \rightarrow \text{NH}_4 \rightarrow \text{Rb}^+$ leads to insignificant changes in λ_{01} , λ_{02} , B_1 and B_2 and a decrease in n_i by approximately 0.02 and 0.03.

It was found that the baric increase in the absolute value of the RI is due to a decrease in the effective power of the UV oscillator and a shift of the effective center of the UV absorption band to the long-wavelength region of the spectrum with a speed of $d\lambda_{0i}/d\sigma_m = 5 - 7 \times 10^{-3}$ nm/bar. If we differentiate (3), we can obtain a relation describing the baric changes in the RI:

$$\frac{dn_i}{d\sigma_m} = \frac{1}{2n_i} \left\{ \frac{\lambda^2 \lambda_{0i}}{\lambda^2 - \lambda_{0i}^2} \left(\frac{dB_1}{d\sigma_m} \lambda_{01} + \frac{2B_1 \lambda^2}{\lambda^2 - \lambda_{01}^2} \frac{d\lambda_{01}}{d\sigma_m} \right) \right. \\ \left. + \frac{\lambda^2 \lambda_{02}}{\lambda^2 - \lambda_{02}^2} \left(\frac{dB_2}{d\sigma_m} \lambda_{02} - \frac{2B_2 \lambda^2}{\lambda^2 - \lambda_{02}^2} \frac{d\lambda_{02}}{d\sigma_m} \right) \right\}. \quad (8)$$

It is considered that mechanical contact changes the forces of the oscillators, and this causes a shift of the corresponding effective centers of the absorption bands.

In this work, changes $d\lambda_{02}/d\sigma_m$ and $dB_2/d\sigma_m$ are neglected, since the effective center of the absorption band λ_{02} of the studied RS crystal is located in the far-IR region of the spectrum. Then, under the condition $dn_i/d\sigma_m > 0$, we can write:

$$\frac{d\lambda_{0i}}{d\sigma_m} > -\frac{\lambda_{0i}(\lambda^2 - \lambda_{0i}^2)}{2B_i \lambda^2} \frac{dB_i}{d\sigma_m}. \quad (9)$$

That is, by the nature of the baric changes in the RI, it is possible to establish the nature of the changes in the oscillators, which are decisive for the refractive properties of the crystal. In general, the anisotropy of electronic polarization corresponds to the anisotropy of the refractive indices ($\alpha_x > \alpha_z > \alpha_y$) (Table 1).

We see that pressures $\sigma \sim 100$ bar cause an increase in the parameter α_i on average by $(1 - 3) \times 10^{-26} \text{ cm}^3$. This value coincides with the baric changes in the volume and linear dimensions of the sample along the direction of compression, which can be obtained based on Hooke's law:

$$\left(\frac{\Delta l}{l_0}\right)_i = s_{im}\sigma_m. \quad (10)$$

Here $(\Delta l/l_0)_i$ are the coefficients of relative elongation, and s_{im} are the coefficients of the elastic compliance tensor.

From formula (10), it is estimated that the coefficients $\Delta l/l_0 \sim 10^{-4}$ for pressures $\sigma_m \sim 100$ bar and values of $s_{im} \sim 10^{-6}$ bar $^{-1}$.

From the relation (6), we can obtain the following expression:

$$\frac{dR}{d\sigma} = -\left(\frac{\mu}{\rho^2} \frac{n^2 - 1}{n^2 + 2} \frac{d\rho}{d\sigma}\right)_n + \left[\frac{\mu}{\rho} \frac{6n}{(n^2 + 2)^2} \frac{dn}{d\sigma}\right]_N, \quad (11)$$

which allows us to find the contributions from the terms with derivatives $\partial\rho/\partial\sigma$ and $\partial n/\partial\sigma$ to the baric changes in the refraction R_i , provided that the values of n and N are constant during the corresponding experiment. If we use the known numerical data for the RS crystal: $\mu = 267$ g/mol, $\rho \sim 3613$ kg/m 3 , $\partial\rho/\partial\sigma \approx s_{im} = 0.5 \times 10^{-10}$ Pa $^{-1}$, $n_i = 1.52$ and $\partial n/\partial\sigma \approx 5 \times 10^{-6}$ bar $^{-1}$, we can obtain that the first term is approximately equal to 2×10^{-4} bar $^{-1}$, while the second is 4.8×10^{-4} bar $^{-1}$. This indicates that the geometric factor is $\sim 28\%$ of the total baric increase in the refraction R .

In the case of neglecting the IR oscillator, the following contributions to the baric changes in the refractive indices can be obtained from relation (8):

$$\begin{aligned} \frac{\partial n}{\partial\sigma} &\approx \frac{1}{2n} \cdot \frac{e^2}{\pi m c_0^2} \left\{ \frac{\lambda^2 \lambda_0^2}{\lambda^2 - \lambda_0^2} \left[f \frac{\partial N}{\partial\sigma} + N \frac{\partial f}{\partial\sigma} \right] + \frac{2Nf\lambda_0\lambda^4}{(\lambda^2 - \lambda_0^2)^2} \frac{\partial\lambda_0}{\partial\sigma} \right\} = \\ &= 0.03 \frac{\partial f}{\partial\sigma} + 10^{-7} f + 3 \cdot 10^{-6} f \frac{\partial\lambda_0}{\partial\sigma}. \end{aligned} \quad (12)$$

Here it is taken into account that the coefficients B_1 and B_2 have the content of polarizabilities and are related to the oscillator strength by the following relations:

$$B_1 = \frac{N_{01} e_1^2 f_1}{\pi c_0^2 m_1^*}; \quad B_2 = \frac{N_{02} e_2^2 f_2}{\pi c_0^2 m_2^*}. \quad (13)$$

Here N_{01} is the number of active particles per unit volume, $e_{1,2}$ and $m_{1,2}^*$ – the charges and effective masses of the oscillators, c_0 – the speed of light in vacuum. From the relation (12) we see that the main contribution to the baric changes of the RI is from the first term $\partial f/\partial\sigma$.

Baric changes of the RI $n_i(\sigma)$ make it possible to estimate the changes in the width of the forbidden band in accordance with the Moss relation [23]:

$$n^4 E_g = \text{const.} \quad (14)$$

If we differentiate the last expression, we obtain:

$$\frac{\partial E_g}{\partial\sigma} = -\frac{4}{n} E_g \frac{\partial n}{\partial\sigma}. \quad (15)$$

If we use the obtained values of the baric changes n_i ($\partial n / \partial \sigma \sim 10^{-6}$ bar $^{-1}$ (Fig. 1), $n_i \sim 1.5$ and $E_g \sim 4.9$ eV), we can estimate the corresponding changes in the width of the forbidden band $\partial E_g / \partial \sigma \sim 1.31 \times 10^{-5}$ eV/bar.

The work also analyzes the baric changes λ_{0i} , B_{1i} and B_{2i} based on the baric dependences of the RI $n_i(\sigma)$ of the studied crystals. For this purpose, the formula (3) was differentiated, which allowed us to obtain the following relation:

$$\frac{dn_i(\lambda, \sigma)}{d\lambda} = -\frac{B_{1i}\lambda_{0i}^4\lambda}{n_i(\lambda^2 - \lambda_{0i}^2)^2} - \frac{\lambda B_{2i}}{n_i}. \quad (16)$$

It was established that the contributions from UV oscillators to the dispersion changes $n_i(\lambda)$ of RS crystals decrease with increasing wavelength, and a significant anisotropy of the contributions from UV and IR oscillators was revealed. Thus, at room temperature, the contributions to the dispersion changes n_i from IR oscillators for $\lambda = 500$ nm are 68.1 % (X-direction) and 81.3 % (Z-direction). Under the action of uniaxial pressure, the contributions from UV oscillators decrease, and from IR – increase. For example, in the spectral region of 700 nm, in the case of increasing uniaxial load from 0 to 200 bar, the contributions from IR oscillators increase from 63.1 % to 66.4 % (Z-direction) (Table 2). At the same time, uniaxial pressures $\sigma_m = 200$ bar shift λ_{0i} to the short-wavelength region of the spectrum $\Delta\lambda_{0x} = 0.8 \dots 1.5$ nm, $\Delta\lambda_{0z} = 1.3 \dots 1.9$ nm.

The change in the effective oscillator strength in this pressure range does not exceed 1 %. Thus, the position of the effective absorption bands is more sensitive to the action of uniaxial pressures than the effective forces of the corresponding oscillators. The application of uniaxial pressures leads to a change in the contributions to the dispersion and temperature dependences $n_i(\lambda, T)$, and this change is not always unambiguous.

Uniaxial pressures cause an increase in contributions from IR oscillators by 2...5 %, which decreases with increasing temperature. This behavior of contributions from IR and UV under the action of different mechanical loads is due, first, to the baric dependence of the optical isotropic point. It was previously shown that for different directions of uniaxial compression, the optical isotropic point moves to a different spectral range, and its existence in any case is determined by the competition of IR and UV oscillators. In general, uniaxial pressures lead to a slight increase in contributions from IR oscillators, which decreases with increasing temperature. With increasing temperature, the increase in contributions from IR oscillators is insignificant – by 1–2 %. Uniaxial pressure σ_z leads to an increase in contributions from IR oscillators by 2–5 %, which decreases with increasing temperature.

The baric variation of the refractive indices of RS crystals is caused by structural changes in the crystal under the action of uniaxial compression. It is known that at room

Table 2. Percentage ratio between contributions from ultraviolet and infrared oscillators to spectral and baric changes in refractive indices of Rb_2SO_4 crystals

$\sigma = 0$ bar								$\sigma = 200$ bar							
300 nm				500 nm		700 nm		300 nm				500 nm		700 nm	
	UV	IR		UV	IR		UV	IR		UV	IR		UV	IR	
X	88.8	11.2	41.4	58.6	21.3	78.7	84.3	15.7	39.4	60.1	20.2	79.8			
Y	90.3	9.7	56.7	43.3	37.9	62.1	83.2	16.8	54.5	45.5	35.3	64.7			
Z	88.7	11.3	55.4	44.6	36.9	63.1	81.7	18.3	55.8	44.2	33.6	66.4			

temperature, the crystal structure is described by the space group symmetry *Pmcn*. In this phase, the tetrahedral SO_4^{2-} groups are somewhat distorted. The "average" spatial structure of RS at room temperature can be represented as follows: the basic orientational unit cell consists of SO_4^{2-} groups, each of which oscillates between three possible equilibrium configurations, defined by the position of the "apical" oxygen atom. The probability of a particular configuration depends solely on the oxygen atom's position, and the distortion of the two nonequivalent ions differs significantly. In general, the structure of the RS crystal in the paraelectric phase can be considered as a partially disordered state with respect to small rotations of SO_4 groups, mainly around the pseudo-hexagonal X-axis [18, 24].

CONCLUSION

In the work, Rb_2SO_4 crystals of good optical quality were synthesized, a crystallographic setup was set up, and the dispersion of the refractive indices $n_x(\lambda)$ at room temperature for different directions of uniaxial compression with a value of $\sigma_m \sim 100$ bar was studied using the Obreimov immersion method. It was found that the dispersion $n_i(\lambda)$ of this crystal is normal $\partial n/\partial\lambda < 0$ (), with an approach to the edge of the fundamental absorption $n_i(\lambda)$ it increases rapidly, and the following relations exist between the refractive indices: $n_x \geq n_z > n_y$ and $dn_x/d\lambda > dn_z/d\lambda > dn_y/d\lambda$.

The analysis of baric changes in the main refractive indices $n_i(\sigma_m)$ of a rubidium sulfate crystal was carried out and it was found that uniaxial pressure does not change the character of the curves $n_i(\lambda)$, but only the magnitude of the dispersion $\partial n_i/\partial\lambda$. It was found that the baric increase in the refractive index is mainly due to a change in the oscillator parameters (~ 72 %) due to a change in the band gap width E_g and a long-wave shift of the maximum of the ultraviolet absorption band and the density of effective oscillators (~ 28 %) of the crystals, as well as a decrease in the effective power of the ultraviolet oscillator and a shift of the effective center of the ultraviolet absorption band to the long-wave portion of the spectrum.

The baric changes in the specific refraction R_i , the electronic polarizability α_i (for the light wavelength $\lambda = 500$ nm), as well as the crystal-optical parameters (positions of the effective centers of the ultraviolet and infrared oscillator bands, as well as the effective forces of the corresponding oscillators) of Rb_2SO_4 crystals at room temperature were calculated. It was found that uniaxial pressures $\sigma \sim 100$ bar cause an increase in the electronic polarizability on average by $(1-3) \times 10^{-26} \text{ cm}^3$, which coincides with the baric changes in the volume and linear dimensions of the sample along the compression direction. In general, the anisotropy of the electronic polarizability corresponds to the anisotropy of the refractive indices ($\alpha_x > \alpha_z > \alpha_y$).

Using the experimentally obtained values of the refractive indices, their baric changes, and the band gap width, the baric changes in the band gap width $\partial E_g/\partial\sigma$ were estimated to be $\sim 1.31 \times 10^{-5} \text{ eV/bar}$.

An analysis of the baric changes in the crystal-optical parameters was carried out and it was found that uniaxial pressures cause an increase in the contributions from infrared oscillators by 2...5 %, which is caused, first of all, by the baric dependence of the optical isotropic point, and also shift the position of the effective force of the ultraviolet oscillator λ_{0i} to the short-wavelength region of the spectrum. It was found that the position of the effective absorption bands is more sensitive to the action of uniaxial pressures than the effective forces of the corresponding oscillators.

COMPLIANCE WITH ETHICAL STANDARDS

The authors declare that they have no competing interests.

AUTHOR CONTRIBUTIONS

Conceptualization, [VS, VV, VB]; methodology, [VS, VV, IM]; investigation, [VS, VV, VB, RL]; writing – original draft preparation, [VS, RL]; writing – review and editing, [VS, VV, IM, VB, RL]; visualization, [VS, VV, VB].

All authors have read and agreed to the published version of the manuscript.

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РЕФРАКТОМЕТРІЯ ОДНОВІСНО ЗАТИСНУТИХ КРИСТАЛІВ Rb_2SO_4

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АНОТАЦІЯ

Вступ. Показник заломлення (ПЗ) n кристалу є його фундаментальною характеристикою. За наявності експериментально отриманої з високою точністю дисперсії $n(\lambda)$ можна визначити фундаментальні характеристики з використанням аналітичних співвідношень для ПЗ в ділянці прозорості кристалу.

Матеріали та методи. У роботі синтезовано кристали Rb_2SO_4 високої оптичної якості, встановлено кристалографічну орієнтацію за допомогою поляризаційного мікроскопа та коноскопічних фігур, досліджено дисперсію показників заломлення $n_x(\lambda)$ методом занурення Обреїмова при кімнатній температурі для різних напрямків одновісного стиснення з величиною $\sigma_m \sim 100$ бар.

Результати. Виявлено, що дисперсія $n_i(\lambda)$ кристалу Rb_2SO_4 є нормальнюю ($\partial n / \partial \lambda < 0$), одновісний тиск не змінює характеру кривих $n_i(\lambda)$, а лише величину дисперсії $dn_i / d\lambda$. Встановлено, що баричне зростання показника заломлення, головно, зумовлено зміною параметрів осциляторів ($\sim 72\%$) за рахунок зміни ширини забороненої зони E_g і довгохвильового зміщення максимуму смуги ультрафіолетового поглинання та густини ефективних осциляторів ($\sim 28\%$) кристалів. Розраховано баричні зміни питомої рефракції R_i , електронної поляризовності α_i , а також кристалооптичних параметрів кристалів Rb_2SO_4 за кімнатної температури. Виявлено, що одновісні тиски $\sigma \sim 100$ бар спричиняють зростання електронної поляризовності в середньому на $(1 - 3) \times 10^{-26} \text{ см}^3$, що співпадає з баричними змінами об’єму та лінійних розмірів зразка вздовж напряму стискання.

Висновки. Було встановлено, що одноосьові тиски призводять до збільшення внеску від інфрачервоних осциляторів на 2–5 %, насамперед через баричну залежність оптичної ізотропної точки. Вони також зміщують положення ефективної сили ультрафіолетового осцилятора λ_{0i} у бік короткохвильової області спектра. Зміна ефективної сили осцилятора в цьому баричному діапазоні не перевищує 1 %. Було виявлено, що положення ефективних смуг поглинання чутливіші до одноосьових тисків, ніж ефективні сили відповідних осциляторів.

Ключові слова: показники заломлення, одновісне стискання, рефракція, електронна поляризовність, ширина забороненої зони.

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