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THE OPTICAL ABSORPTION IN THE IRRADIATED BY X-RAY AND DEFORMED FUNCTIONAL MATERIALS

The optical absorption in the irradiated by X-ray functional materials with the various values of the preliminary deformation is investigated. The irradiation effect on the dependence of the spectral transmittance coefficient $\tau_\lambda(\lambda)$ on the wavelength at the range of 220...650 nm in LiF crystal with the residual strain of 3,3 % at an irradiation dose range of 0...1057 R has been elaborated. The wavelength localization of the absorption band half-width peak is defined on the base of the presence of the F – centers in irradiated crystals is concluded. It has been found that under the X-ray irradiation at the dose of 400 R the transmittance capacity of samples is reduced, and at the dose range of 800 ... 1057 R the absorption band with a maximum at the wavelength of 248 nm, which was formed in connection with the introduction of F- centers in crystals has been clearly observed. On the basis of the examined spectrum of $\tau_\lambda(\lambda)$ in the range 220...650 nm for LiF crystals with the residual strain of 0,4 and 0,65 % and irradiated with X-rays to a dose of 1057 R it has been concluded that radiation-induced defects by their physical nature are F-centers. Based on the dispersion ratio of Smakula, it has been calculated the volume density calculation of F-centers N_F in LiF crystals. For samples with LiF with ε = 3,3 % the values N_F were $5,21\cdot10^{15}$ and $5,28\cdot10^{15}$ sm $^{-3}$ for dose 800 and 1057 R respectively, and for LiF crystals with deformations of 0,4 and 0,65 % at X-rays dose of 1057 R, the value N_F were equal to $8,49\cdot10^{15}$ and $10,85\cdot10^{15}$ sm $^{-3}$ respectively.

Keywords: *residual strain, radiation defects, color centers, transmittance coefficient , dispersion ratio of Smakula.*

Introduction

It is known [1] that when the crystal is exposed to X-ray irradiation, the main part of its energy is spent on the creation of electronic excitations. In the presence of these excitations in the vicinity of anion vacancies, due to the localization of electrons on them, appear electron color centers. In the simplest case, these are F- centers [2], then, with the accumulation of the radiation dose in the crystal, the combination of F-centers into more complex units are possible. For example, if there are two adjacent F- centers, F_2 (M) - centers appear, three - F_3 (R) - centers and etc. To study the mentioned and other types of radiation defects the absorption method [1, 2] is widely used. It is based on measuring of dependences from the wavelength of the spectral transmittance index $\tau_\lambda(\lambda)$ in the UV and visible range of the spectrum. Having the color centers in the crystal at the specified dependences, the areas where transmission is minimal have been traced – namely, the so-called absorption bands. From the data on the absorption band (in particular, its localization on the wavelength axis) information about the type of defect as well as their amount has been obtained. It should also be emphasized that the most convenient of ionic crystals for optical studies are crystals LiF, in which color centers are highly resistant to photoexcitation and are stored at room temperature for a long time [1].

The aim of this paper is to obtain qualitative and quantitative information about the effect of X-ray irradiation and dislocation structure to the optical properties of the modern functional materials.

Materials and Methods of the Research

For the experiment the samples LiF with residual deformations 0,4; 0,65 and 3.3 % have been used. After reaching the preliminary sizes, samples were grounded and polished to achieve the level of plane paralell ± 1mkm/sm that was controlled by the IKV optimeter. To remove the internal stresses, arising as a result of mechanical processing, the samples were annealed for ~ 12 hours in a muffle furnace MP- 2UM oven at ~ 0.8 T_{melt} with further slow cooling to room temperature. Crystals deformation has been performed with the compression at on a tensile testing machine type "Instron" with the speed index of ~ 10^{-5} s^{-1}. The geometric dimensions of the samples before and after loading have been monitored by comparator IZA- 2. The irradiation of crystals by X-ray has been performed at the same apparatus (URS- 55) and at the same mode (40 kV, 10 mA) as in previous works. The total exposure time of the crystals was 160 minutes, that at the radiation dose rate at the location of the researched crystals 0,11 R / s corresponded to a radiation dose 1057 R. The optical experiment has been carried out on the SF-26 spectrophotometer in the wavelength range 220...650 nm.

Results and Discussion

Figure 1 shows the measurement results of spectral coefficients of transmission τ_λ at wavelengths range 220...650 nm on LiF crystals having a residual deformation of 3.3 % at the irradiation dose range of 0...1057 R. As it can be seen from Fig.1 for unirradiated crystals the value τ_λ monotonously increase with the increase of the wavelength (curve 1). In the case of crystal irradiation with the dose of 400 R the curve $\tau_\lambda(\lambda)$ remains virtually unchanged, but the transmittance capacity of samples is significantly reduced (curve 2).

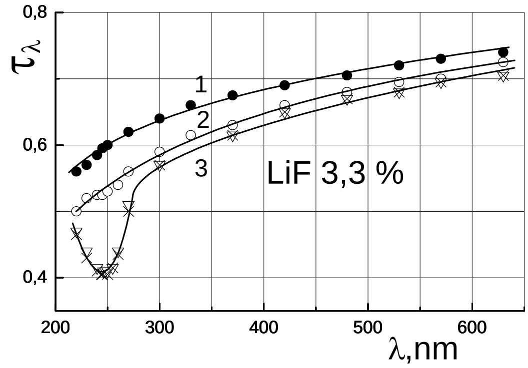

Fig.1. Dependences of the spectral transmittance coefficient of the wavelength in LiF crystals on different doses of irradiation: curve 1 - unirradiated crystal, 2 - irradiation dose of 400 R , 3 - irradiation dose of 800 R (points ∇) and 1057 R (point X)

With the increase of the radiation dose up to 800 R (curve 3 - experimental points marked ∇) a pronounced absorption band has been observed, which corresponds to the minimum on the curve $\tau_\lambda(\lambda)$, which lies at a wavelength of approximately 248 nm. At other segments of the wavelength, the mode of dependence $\tau_\lambda(\lambda)$ does not change. The indicated character of curve $\tau_\lambda(\lambda)$ behavior is preserved even in the case that a dose of X-ray irradiation is increased to 1057 (see curve 3 - experimental points are marked ×).

The reported features observed in the experiment, allow to make some conclusions. The presence of the absorption bands indicates the presence of color centers in crystals. Since for ionic crystals the bands borders are fairly well researched, it is possible to mark, that in the measured samples there are clearly presented, having the simplest configuration, electronic color centers - F-centers, the minimum on the curve $\tau_\lambda(\lambda)$ (for which the maximum of the attenuation) is at the wavelength $\lambda_{max} \approx$ 248 nm [1]. It has been also noted that there is no evidence for the presence of F_2 and F_3 –centers in samples the given curves do not show, as in the vicinity of $\lambda_{max} \approx$ 443 nm for F_2- centers and $\lambda_{max} \approx$ 307 and 377 nm for different types of F_3- centers [1-3] there have not been found any nonmonotonicies. The results of measuring the dependency $\tau_\lambda(\lambda)$ for crystals LiF with deformation 0,4 and 0,65 % are presented in Fig. 2. It is evident that for crystals with identified ε in the vicinity of $\lambda_{max} \approx$ 248 nm the absorption bands are clearly seen. It can be noted that at the transition from a small ε to a larger, the transmittance capacity of samples decreases and the rate of this decline is visually the same at all the considered spectral ranges. It also shows that at the range 300...650 R the spectral transmittance monotonically increases with the increase of the wavelength.

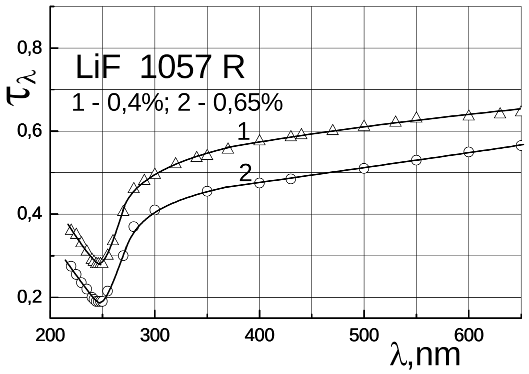

Fig.2. Dependences of the spectral transmittance coefficient on the wavelength at irradiated to a dose of 1057 R LiF crystals with values of preliminary deformation of 0,4 and 0,65 %

To determine the amount of occurred under the action of radiation color centers, the Smakula dispersion relation has been used [4-6], that allows to determine the concentration of F- centers by the parameters of the absorption band. This ratio is widely used in optical radioactive material science, and with its help a number of the experimental results have been processed. The theoretical test of the Smakula relation has been undertaken by the author [6], who investigated this problem at the level of quantum electrodynamics based on the consideration of various forms of absorption bands - Lorentz and Gauss, and came to a result similar to [5].

Smakula dispersion ratio, allowing to indicate the concentration of color centers in the crystal N_F has the form [4-6]:

$$N_F = \frac{A}{f} \cdot \frac{n}{(n^2+2)^2} \cdot K_m \cdot \Delta E \qquad (1)$$

where A = $1{,}31 \cdot 10^{17}$ is a numerical coefficient, which is valid for Lorentz form of absorption band, f - oscillator strength (equal to 0,8 for a Lorentz band form), n = 1,42 for LiF [7] - the refractive index of unexcited crystal in area $\lambda_{max} \approx$ 248 nm, K_m - maximum value of the attenuation index, ΔE - half-width of the band, determined by the width of the absorption line at its half-height [4-6].

To determine the parameters K_m and ΔE from the data Fig. 1 it is necessary to use the ratio [5], valid for the case when light is passing through a plane-parallel layer of substance (see Fig. 3) and taking into account the reflection losses from the two faces of the sample ($\Phi_{\rho 1} + \Phi_{\rho 2}$):

$$\tau = (1-\rho)^2 \cdot e^{-k\ell} \qquad (2)$$

where ^{2} - transmittance coefficient of the crystal, $^\circ = (\frac{n-1}{n+1})^2$ - the coefficient of reflection, K – attenuation index, ℓ - the optical path of light in a substance. It should be noted that the ratio (2) ignores the multiple rereflection in samples.

However, taking into account that for LiF crystals the reflection does not exceed 3 %, the consideration of additional contributions into total sample transmission of the passed to the multipath detector rereflected signals is not required, and our evaluation has confirmed that strict accounting of the entire series of passed signals, changes the value ^{2} to the fractions of the percent, which does not put the specified result of the transmission beyond the error measurements on the spectrophotometer SF-26.

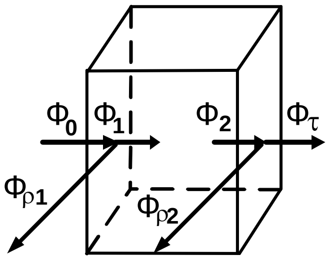

Fig. 3. Light passing through the sample

Taking into consideration $(1-\,^\circ)^2 = 0{,}94$ the attenuation index for crystals can be calculated by the formula:

$$K = [2{,}3 \cdot \log(0{,}94/^2)]/\ell, \qquad (3)$$

where $\log(0{,}94/^2)$ - is the optical density of the sample. Therefore, having dependency $\tau_\lambda(\lambda)$ and the known value ℓ the dependence $K_\lambda(\lambda)$ can be determined.

The results of dependence calculation of the spectral index of the attenuation function from the wavelength for LiF crystals with the size of the residual strain of 3,3% and radiation doses 800 and 1057 R are shown in Fig . 4.

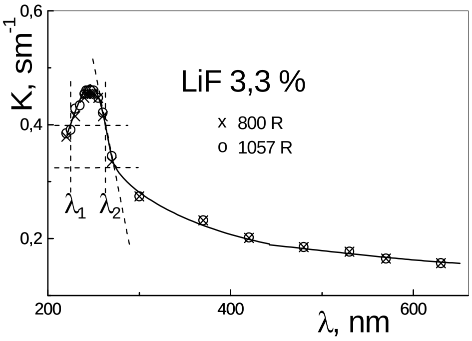

Fig. 4. Dependences of the attenuation index on the wavelength in crystals LiF with ε = 3,3 % for the irradiation doses of 800 and 1057 R. The dashed lines show the method of determining the half-width boundaries of the absorption band

In this figure, the absorption band, caused by the presence of F-centers with a distinct peak at the wavelength $\lambda \approx 248$ nm has been clearly traced. At the same figure the dashed lines shows how the boundaries λ_1 and λ_2 of the half-width have been determined. The band half-width is required to calculate the value of N_F by the ratio (1) and was determined by the well known formula $\Delta E = 1241 \cdot (\frac{1}{a_1} - \frac{1}{a_2})$ [8] and was approximately 0,8 eV, which corresponds well to the literature data for LiF at 300 K [1-3].

The calculation of the color centers N_F concentration for LiF crystals with ε = 3,3 % and radiation doses of 800 and 1057 R gave values of $5{,}21 \cdot 10^{15}$ and $5{,}28 \cdot 10^{15}$ sm $^{-3}$ respectively. Similarly there were constructed and processed dependences $K_\lambda(\lambda)$ for crystals with LiF with ε = 0,4 и 0,65 %, irradiated to a dose of 1057 R.

Calculating N_F, the value of $8{,}49 \cdot 10^{15}$ and $10{,}85 \cdot 10^{15}$ sm^{-3} for LiF samples with ε 0,4 и 0,65 % respectively have been obtained. It can be concluded that differences in the dislocation structure of the samples at the same dose of their irradiation in these experimental conditions do not affect the type of the observed color centers, whereas the quantitative results are changed [9-10].

Conclusions

The irradiation effect on the dependence of the spectral transmittance coefficient $\tau_\lambda(\lambda)$ on the wavelength at the range of 220...650 nm in LiF crystal with the residual strain of 3,3 % at an irradiation dose range of 0...1057 R has been elaborated. It has been found that under the X-ray irradiation at the dose of 400 R the transmittance capacity of samples is reduced, and at the dose range of 800 ... 1057 R the absorption band with a maximum at the wavelength of 248 nm, which was formed in connection with the introduction of F- centers in crystals has been clearly observed. On the basis of the examined spectrum of $\tau_\lambda(\lambda)$ in the range 220...650 nm for LiF crystals with the residual strain of 0,4 and 0,65 % and irradiated with X-rays to a dose of 1057 R it has been concluded that radiation-induced defects by their physical nature are F-centers. Based on the dispersion ratio of Smakula, it has been calculated the volume density calculation of F- centers N_F in LiF crystals. For samples with LiF with ε = 3,3 % the values N_F were $5{,}21 \cdot 10^{15}$ and $5{,}28 \cdot 10^{15}$ sm $^{-3}$ for dose 800 and 1057 R respectively, and for LiF crystals with deformations of 0,4 and 0,65 % at X-rays dose of 1057 R, the value N_F were equal to $8{,}49 \cdot 10^{15}$ and $10{,}85 \cdot 10^{15}$ sm $^{-3}$ respectively.

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ОПТИЧНЕ ПОГЛИНАННЯ У ОПРОМІНЕНИХ Х-ПРОМЕНЯМИ ПРОДЕФОРМОВАНИХ ФУНКЦІОНАЛЬНИХ МАТЕРІАЛАХ

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Вивчено оптичне поглинання випромінювання на опромінених Х-променями функціональних матеріалах з різними величинами попередньої деформації. Визначено напівширину смуги поглинання та локалізацію її максимуму, на підставі чого зроблено висновок щодо наявності F-центрів у опромінених кристалах. За формулою Смакули визначено об'ємну густину вказаних радіаційних дефектів.

Ключові слова: *попередня деформація, радіаційні дефекти, центри забарвлення, коефіцієнт пропускання, дисперсійне співвідношення Смакули.*

ОПТИЧЕСКОЕ ПОГЛОЩЕНИЕ В ОБЛУЧЕННЫХ Х-ЛУЧАМИ ПРОДЕФОРМИРОВАННЫХ ФУНКЦИОНАЛЬНЫХ МАТЕРИАЛАХ

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Изучено оптическое поглощение излучения на облученных Х-лучами функциональных материалах с различными величинами предварительной деформации. Определена полуширина полосы поглощения и локализация ее максимума, на основании чего сделан вывод о присутствии F-центров в облученных кристаллах. По формуле Смакулы определена объемная плотность указанных радиационных дефектов.

Ключевые слова: предварительная деформация, радиационныеі дефекты, центры окраски, коэффициент пропускания , дисперсионное соотношение Смакулы.