DEPENDENCE OF ELECTRONIC COLOR CENTER CONCENTRATION ON THE STATE OF IRRADIATED LiF CRYSTAL DISLOCATION STRUCTURE

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The optical radiation absorption has been investigated for LiF crystals preliminary deformed to the level of 0.155 and 1.5% under irradiation to a dose of 1057 R. A conclusion on the presence of F-centers in irradiated crystals is drawn. The volume density of the observed radiation defects is evaluated. Basing on the experimental data of the present and previous papers the deformation dependences of the spectral damping coefficient K_λ and the concentration N_F of F centers were investigated.

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INTRODUCTION

The paper presents overall results of recent publications [1–3] on the nature of radiation defects in irradiated LiF crystals. The investigations have been undertaken to find out the effect of the irradiation dose and the degree of preliminary deformation ε on the dependences of the radiation-transmission coefficient τ_λ in the wavelength range of 220…650 nm. For this purpose the optical absorption method has been applied. In the crystal irradiated with a dose of about 500 R the appearance of absorption bands due to the formation of F-centers was observed. It has been concluded that in the spectral range of the irradiation dose interval between 0 and 1057 R, from a possible variety of different electronic color centers arising in the crystals under irradiation, only F-centers are presented. From the half-widths of the absorption band and its localization on the wavelength axis within the framework of the Smakula theory the volume density N_F of F-centers in the crystals was calculated. In particular, in the case of LiF irradiation with a dose of 1057 R the calculated value of N_F was $1.15\cdot10^{16}$ cm^{-3} for $\varepsilon = 0.8\%$ [1]; $8.34\cdot10^{15}$ and $10.34\cdot10^{15}$ cm^{-3} for $\varepsilon = 0.3$ and 1.2%, respectively [2]; $8.49\cdot10^{15}$; $10.85\cdot10^{15}$ and $5.28\cdot10^{15}$ cm^{-3} for $\varepsilon = 0.4$; 0.65 and 3.3% respectively [3]. In paper [3] a nonmonotonic character of the color center concentration dependence on the dislocation structure of samples was noticed, therefore, as an urgent problem, it has been intended to study in more detail the functional dependence of $N_F(\varepsilon)$.

It will be recalled that investigations [1–3] were carried out to identify the radiation defects playing a role of weak centers of pinning of dislocations in the series of acoustic experiments [4], and that overall optical-acoustic results give a complete picture of physical processes proceeding in the crystals under X-ray irradiation.

An objective of the present paper is to supplement and complete the available information about the preliminary deformation value influence on the localization of spectral characteristics of the transmission coefficient $\tau_\lambda(\lambda)$ in irradiated LiF crystals. This allows us to analyze the dependences of the spectral damping coefficient K_λ and F-center concentration N_F on ε.

MATERIALS AND EXPERIMENTAL TECHNIQUES

For experiments LiF crystals having a purity of 10^{-4} wt.%, residual deformation of 0.155 and 1.5%, approximate dimensions $16\times16\times29$ and $16\times16\times25$ mm^3, respectively, were prepared by gouging along cleavage plane {100}. The level of the sample flatness, ± 1 μm/cm, achieved by grinding and polishing, was controlled with an optimeter IKV. The samples were annealed for 12 hours in a muffle furnace MP-2UM at temperature of about 0.8 T_{melt} and after that slowly cooled to room temperature. Crystals were deformed by compression with the speed index of about 10^{-5} s^{-1} in the "Instron" tensile testing instrument. The yield strength of the crystals, an exact value of which is necessary for deformation time reading, was recorded on the chart of the recorder KSP-4. Geometric dimensions of the samples were monitored with a comparator ISA-2. X-ray irradiation of the crystals has been performed using the same apparatus URS-55 (40 kV, 10 mA) as in the previous experiments. The total exposure time was 160 min that at a dose rate of 0.11 R/s, in the site of crystals being investigated, corresponded to the irradiation dose of 1057 R. The dependences $\tau_\lambda(\lambda)$ for the crystals having different ε values have been measured with a spectrophotometer SF-26 in the wavelength interval of 220…650 nm. According to the meter certificate in the spectral range of 220…350 nm a deuterium lamp DDS-30 was used as a lighter, and in the range of 350…650 nm an incandescent lamp OP-33-0.3 was used. Over the entire measurement range a surmyan-cesium photocell F-17 was applied as a radiation detector.

RESULTS AND DISCUSSION

Fig. 1 shows the curves of the spectral transmittance τ_λ in the wavelength interval of 220…650 nm obtained for the LiF crystals having a residual deformation of 0.155 and 1.5% at an irradiation dose of 1057 R.

It is seen from Fig.1 that in the case of the crystals with the indicated values of ε the distinct absorption bands near $\lambda \approx 248$ nm take place. It is also obvious that at the transition from 0.155 to 1.5% the transmission capacity of the samples slightly decreases but there is no evident qualitative changes in the shape of the $\tau_\lambda(\lambda)$ curve.

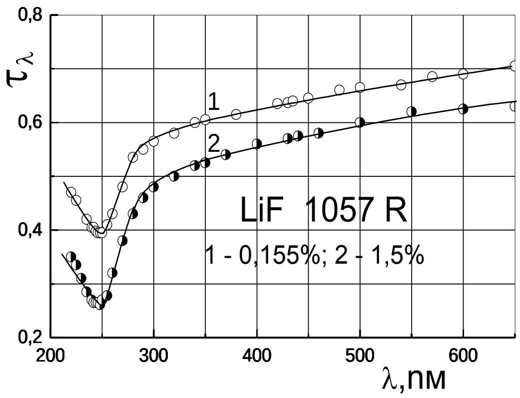

Fig. 1. Spectral transmittance as a function of the wave length in the LiF crystals preliminary deformed to 0.155 and 1.5% and irradiated to 1057R

The presence of the absorption bands in the vicinity of $\lambda \approx 248$ nm and the monotonic increase of the $\tau_\lambda(\lambda)$ curves in the range of 300…650 R indicates the presence of F-centers in the irradiated crystals [5] and on the absence of more complex configurations of the color centers giving the bands at $\lambda_{max} \approx 443$ nm (F_2-centers) and at $\lambda_{max} \approx 307$ and 377 nm (different types of F_3-centers) [6].

Basing on the experimental results the volume density N_F of electronic color centers was calculated. For this the Smakula dispersion relation [7] was used to determine the F-center concentration by the absorption band shape.

According to [7] the above relation is written in the following form:

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

where $A = 1.31 \cdot 10^{17}$ is the numerical coefficient being valid for the Lorentzian shape of the absorption band, f – oscillator strength (equal to 0,8 for the Lorentzian shape of the absorption band), n = 1,42 for LiF [8] – refractive index of the nonexited crystal in the region of $\lambda_{max} = 248$ nm, K_m – maximum value of the damping factor, ΔE – band half-width determined by the absorption line full width at half-maximum [9].

The value of was determined K_m using the relation of [9]:

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

where τ is the crystal transmission coefficient, $\rho = (\frac{n-1}{n+1})^2$ – reflection coefficient, K – damping coefficient, ℓ – radiation optical path in the substance. Since $(1-\rho)^2 = 0{,}94$ it is evident that using the relationship $\tau_\lambda(\lambda)$ and the known value of ℓ we can determine the relationship $K_\lambda(\lambda)$:

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

where $\log(0{,}94/\tau)$ is the optical sample density.

The calculated dependences of the spectral damping coefficient on the wave length for the LiF crystals with residual deformation values 0,155 and 1.5% and irradiation dose of 1057 R are shown in Fig. 2,a,b.

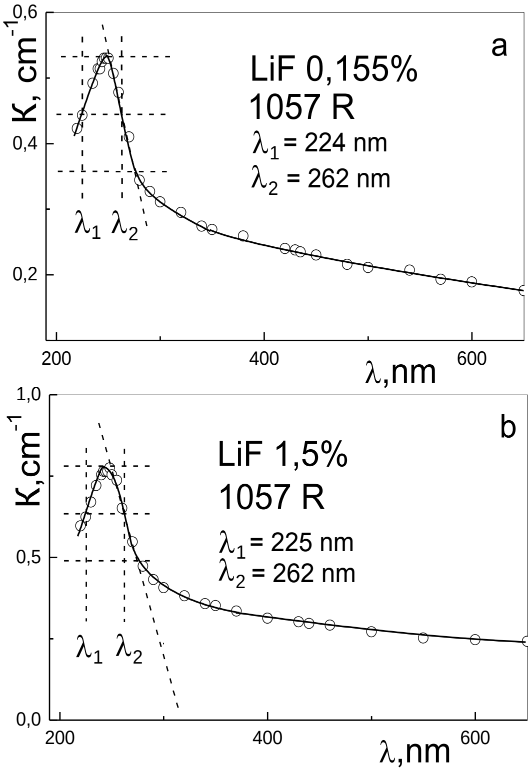

Fig. 2. Spectral damping coefficient as a function of the wave length in the LiF crystals with preliminary deformation values 0,155% (a) and 1,5% (b) irradiated with a dose of 1057R. The dotted lines show the method for determining the edges of the absorption band half-width

From Fig. 2 the values of K_m and ΔE can be determined by the parameters of the band and its localization on the wave length axis. The band half-width was calculated by the formula $\Delta E = 1241 \cdot (\frac{1}{\lambda_1} - \frac{1}{\lambda_2})$ [9]. The values of the band edges were determined by the method demonstrated in Fig. 2. The values of ΔE for the crystals with ε equal to 0.155 and 1.5% were 0.8 and 0.78 eV respectively, that is in good accord with the literature data for LiF at 300 K [5].

The values of N_F calculated by equation (1) for the LiF crystals with ε equal to 0. 155 and 1.5 % irradiated with a dose of 1057 R were $6{,}135 \cdot 10^{15}$ and $8.7 \cdot 10^{15}$ cm^{-3} respectively.

The results reported here and the data of [1–3] were used to find out the deformation dependence of the maximum of the crystal damping coefficient in the interval of preliminary deformation degrees of 0.155…3.3%.

As it has been assumed in [3] the dependence $K_m(\varepsilon)$ is nonmonotonic. The peak in the curve is observed near 0.7…0.8%. It is known from [4] that the indicated values of ε for LiF characterize a peculiar state of the crystal being deformed, namely, when the dislocations are maximally unpinned from their stoppers and the process of their repinning, due to the interaction between the primary dislocations and "forest" dislocations, does not begin yet.

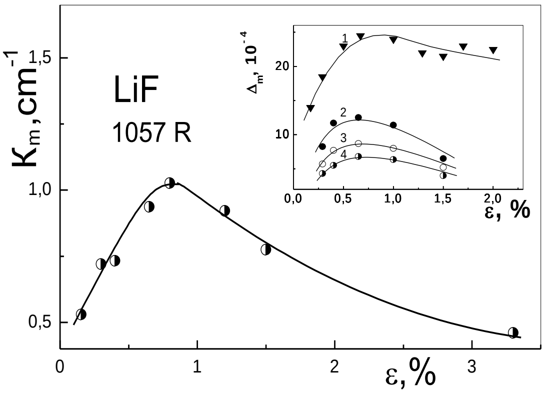

Fig. 3. Maxima of the spectral damping coefficient as a function of the preliminary deformation value in the LiF crystals irradiated to a dose of 1057 R. The inset shows the deformation dependences of a maximum of the dislocation ultrasound damping decrement for unirradiated (1) and irradiated (2–4) LiF crystals [4]

The inset in Fig. 3 shows the dependences of the dislocation damping decrement $\Delta_d(\varepsilon)$ for unirradiated (1) and irradiated (2–4) LiF crystals we have obtained before in [4]. An evident analogy, attracting our attention, is observed in the shape of $K_m(\varepsilon)$ and $\Delta_d(\varepsilon)$ curves. It can be assumed that the acoustic and electromagnetic waves respond similarly to the dislocation crystal structure. Theoretically it is quite possible with taking into account that in a qualitative sense the medium propagation equations are practically identical for both waves. From the results in Fig. 3 it follows that the greater average effective length of the dislocation segment, the higher ultrasound loss and loss of the optic radiation upon traversing material.

To analyze in more detail the dependence given in Fig. 3 and to get information on the process of color center multiplication by deformation we have traced the F-center concentration N_F as a function of the deformation (see Fig. 4).

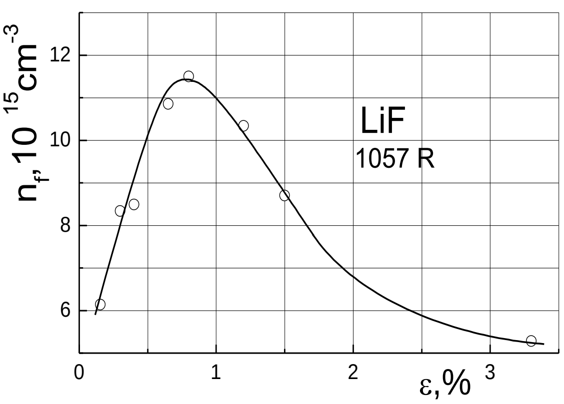

Fig. 4. Concentration of F-centers in the LiF crystals irradiated to a dose of 1057 R as a function of the preliminary deformation

It is clear from the figure that qualitatively the $N_F(\varepsilon)$ curve does not differs at all points from the $K_m(\varepsilon)$ curve that is explained by the direct proportional dependence of these characteristics resulting from Equation (1). It follows from Fig. 4 that the state of maximum unpinning of dislocation segments in the crystal is the most favorable factor for formation of a significant number of F-centers in the crystal.

A picture of the physical processes observed in the irradiated crystals qualitatively can be represented by the following way. In the crystal being irradiated the radiation defects are formed. Dislocations in the crystal play a role of some traps for these defects [10]. The maximum unpinning of dislocations from their stoppers in the region of ε near 0.7…0.8% results in increasing the number of F-centers in the crystal volume without dislocations. Probably this promotes the formation of a great number of free resonators responsible for the optical radiation energy absorption.

CONCLUSIONS

1. The X-ray irradiation effect on the spectral transmittance $\tau_\lambda(\lambda)$ dependence on the wave length in the range of 220…650 nm has been investigated for the LiF crystals with residual deformations of 0.155 and 1.5% irradiated to a dose of 1057 R. The results show that near $\lambda \approx 248$ nm the absorption bands are formed due to the occurrence of F-centers in the crystals.

2. Basing on the Smakula's dispersion relation the calculation of the F-center concentration N_F in the LiF crystals was performed. For the LiF samples with deformations of 0.155 and 1.5% after X-ray irradiation to a dose of 1057 R the values of N_F were $6.135 \cdot 10^{15}$ and $8.7 \cdot 10^{15}$ cm^{-3} respectively.

3. The deformation dependences of the spectral crystal damping coefficient K_λ and the electronic color center concentrations $N_F(\varepsilon)$ with the preliminary deformation level of 0.155…3.3% were determined. The characteristics obtained are nonmonotonic dependences with maxima in the deformation range of 0.7…0.8% characterized by a maximum unpinning of mobile dislocations from the point pinning centers.

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ЗАВИСИМОСТЬ КОНЦЕНТРАЦИИ ЭЛЕКТРОННЫХ ЦЕНТРОВ ОКРАСКИ ОТ СОСТОЯНИЯ ДИСЛОКАЦИОННОЙ СТРУКТУРЫ ОБЛУЧЕННЫХ КРИСТАЛЛОВ LiF

Г.А. Петченко, А.М. Петченко

Изучено оптическое поглощение излучения для облученных до дозы 1057 Р кристаллов LiF с величинами предварительной деформации 0,155 и 1,5%. Сделан вывод о присутствии F-центров в облученных кристаллах, определена объемная плотность указанных радиационных дефектов. На основании экспериментальных данных, полученных в настоящей и предыдущих работах, изучены деформационные зависимости спектрального показателя ослабления K_λ и концентрации F-центров N_F.

ЗАЛЕЖНІСТЬ КОНЦЕНТРАЦІЇ ЕЛЕКТРОННИХ ЦЕНТРІВ ЗАБАРВЛЕННЯ ВІД СТАНУ ДИСЛОКАЦІЙНОЇ СТРУКТУРИ ОПРОМІНЕНИХ КРИСТАЛІВ LiF

Г.О. Петченко, О.М. Петченко

Вивчено оптичне поглинання випромінювання для опромінених до дози 1057 Р кристалів LiF з величинами попередньої деформації 0,155 та 1,5%. Зроблено висновок щодо присутності F-центрів в опромінених кристалах, визначено об’ємну густину вказаних радіаційних дефектів. На підставі експериментальних даних, отриманих у цій та попередніх роботах, вивчено деформаційні залежності спектрального показника ослаблення K_λ та концентрації F-центрів N_F.