JOURNAL OF NANO- AND ELECTRONIC PHYSICS Vol. **10** No 5, 05022(5pp) (2018)
ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ Том **10** № 5, 05022(5cc) (2018)

Empirical Regularities of Change in Dynamic, Acoustic, Structural, Optical and Colorimetric Characteristics of Ionic Crystals with Debye Temperature

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(Received 12 July 2018; published online 29 October 2018)

The paper deals with the possibly establishing a hierarchy of phonon mechanisms of dislocations' attenuation at the Debye temperature in the investigated crystal. For the first time, the reproduction technology of dislocation absorption's frequency spectra of ultrasound in crystals at a known Debye temperature was demonstrated, as well as an algorithm for switching from thermal to structural, dynamic, acoustic, optical and colorimetric characteristics of crystals. There were studied the influence of structural defects of a crystal, in particular, nodes of a dislocation grid and pinning centers in the dislocations of different physical nature on the proposed empirical regularities, and the expediency of their use for samples of ionic crystals with different mechanical states was also grounded.

Keywords: Phonon braking, Dislocation decrement, Deformation, Irradiation, Dislocations, Debye temperature, Attenuation index, Coefficient of dynamic drag, Elastic modules.

DOI: 10.21272/jnep.10(5).05022 PACS numbers: 43.35. + d , 61.80. – x

1. INTRODUCTION

In paper [1] it is noted that in the high-speed motion of dislocations in crystals ($\upsilon \geq 10^{-2}\upsilon_s$, where υ_s is the velocity of sound in the investigated medium), the mobility of dislocations is limited by their interaction with elementary excitations in the crystal (electrons, phonons, etc.). In this case, the action of the viscous medium is taken into account by the coefficient of damping B, which includes the total effect of all braking forces acting on the dislocation. The study of the effect of various factors on parameter B is a fundamental scientific problem of plasticity and strength physics, since studying the mobility of dislocations allows us to describe and predict the process of plastic deformation in crystals, which is important for the creation and modernization of functional elements used in modern devices and systems.

The authors [1, 2] also noted that ion crystals are the most convenient in order to study the phonon braking of the dislocations. Due to the lack of these electronic crystal components, it is convenient to use them both for testing existing and constructing new physical theories, and for the correct study of the phonon component in inhibiting dislocations by the gas of elementary excitations in the pure form.

By analyzing the experimental material obtained for a number of KBr, NaCl, KCl, CsJ, LiF ionic crystals, the author [3] drew our attention to the importance of establishing correlation dependence between the phenomenological parameter Δ_e of the Alschitz-Indenbom's theory [1] and the Debye temperature of the investigated crystal θ.

The mentioned theory [1], operating with experimental data on crystals with different temperatures of Debye, works in such a way, that to identify the phonon mechanisms of inhibition of the dislocations in the investigated crystal, the experimentally obtained dependence of $B(T)$ was reconstructed in the combined coordinates $B(T)/B(\theta) - T/\theta$ and compared with the theoretical profile proposed by the authors [1]:

$$\frac{B(T)}{B(\theta)} = \frac{f_1(\frac{T}{\theta})}{f_1(1)}(1-\Delta_e f_2(1)) + \Delta_e \frac{\theta}{T} f_2(\frac{T}{\theta}), \quad (1)$$

where $f_1(T/\theta)$, $f_2(T/\theta)$, $f_1(1)$, $f_2(1)$ – the theoretical functions given in paper [1] as a graphical form. The high-temperature asymptote to the zero temperatures of the experimental curve $B(T)/B(\theta) - T/\theta$ determines the value of the dimensionless parameter Δ_e. In fact, this parameter adapts the theoretical template [1] to the description of the behavior of a real crystal. By comparing the course of the theoretical and experimental curves, we conclude that the mechanisms of phonon wind and the relaxation of "slow" phonons are effective. The parameters' combination Δ_e and θ shows the entire process of phonon braking of dislocations in a crystal quite clearly. In paper [3], the dependence $\Delta_e(\theta)$ (Fig. 1) on the basis of which the method of predicting the absolute value and temperature of the dynamic inhibition coefficient of dislocations B for any similar ionic crystals was proposed for the five previously studied crystals.

As can be seen from Fig. 1, for any non-investigated crystal (for example, NaF), one can determine the value Δ_e, and then a theoretical dependence of $B(T)/B(\theta) - T/\theta$ can be set at a known Debye temperature.

In addition, it is possible to determine the absolute value of B for any fixed temperature, using another ratio of authors [1]:

$$B = [4 + (\frac{|n|}{G} - 6)^2]\frac{\xi}{b^3}(\frac{\kappa_D b}{2\pi})^5 [f_1(\frac{T}{\theta}) + \lambda_\theta \frac{\theta}{T} \cdot f_2(\frac{T}{\theta})], \quad (2)$$

where n – Murnagan's module, $\xi = h/2\pi$ (h – Plank's constant), $\kappa_D \approx 5/b$ (where b – vector module of Burgers), $\lambda_\theta = \Delta_e \cdot f_1(1)/1 - \Delta_e \cdot f_2(1)$, $|n|/G = 30$ [1].

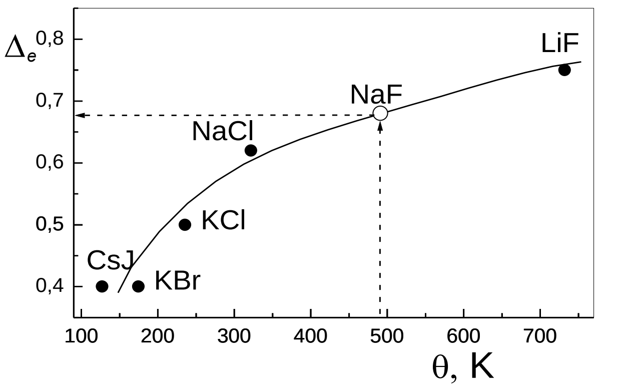

Fig. 1 – Correlation between the phenomenological parameter Δ_e and the Debye temperature θ for ionic crystals [3]. Dashed lines show the determination of the value of Δ_e for the crystal NaF unexplored experimentally

Thus, the method proposed in [3] enables to predict the level of dynamic drag of dislocations due to the Debye temperature in a wide temperature range (from $T/\theta \approx 10$ and above [1]).

The purpose of this work is a comprehensive consideration of factors that can limit the effectiveness of this methodology utilizing. It is also aimed to analyze some new possibilities for the most convenient evaluating and predicting the behavior of fundamental physical characteristics and seeking links between them.

2. EXPERIMENTS, RESULTS AND DISCUSSION

The generation basis for the mentioned methods [3] was an array of experimental data obtained for five ionic crystals – KBr, NaCl, KCl, CsJ, LiF, for which by means of the amplitude-independent viscosity method for the frequency range 7,5-232,5 MHz, the systematic studies were performed on the influence of temperature (in the range 77-300 K) and residual deformation of samples (up to $\varepsilon \approx 2$ %) on the localization of frequency spectra $\Delta_d(f)$ the dislocation decrement of ultrasonic attenuation in crystals.

The technological cycle of preparing all the mentioned crystalline samples was as follows. The comparison specimens under investigation after breaking off were subjected to fine polishing so that the non-parallelism of their working surfaces became approximately 1 μm/cm, which was controlled by means of an IKV-type optimeter. An independent evaluation of the degree of non-parallelism in the system "piezoquartz-gluing-sample" was carried out additionally by means of applying a reference signal of the exponential form to a series of reflected pulses observed on an oscilloscope when the crystal was sounded. To remove the internal strain that could result from mechanical processing of samples, they were annealed for 12 hours in a muffle furnace MP-2UM at a temperature of ~ 0,8 T_{ml} (where T_{ml} – melting temperature), then they are exposed to a subsequent slow cooling to room temperature. For implanting of "light-moving" dislocations into the crystal, it was preliminarily deformed to obtain the required degree of prestrain ε. The output to the required value ε was provided by the accurate fixing of the crystals' flow boundary on the tape of the recorder KSP-4. The working length of the crystal before and after the deformation was controlled by means of IZA-2, the comparator with accuracy to 1 μm. The deformation of the samples was carried out by compressing them with an Instron machine at a speed of ~ 10^{-5}s^{-1}. In this mode, the deformation of the slip line did not occur, and the pockets of etching evenly covered the surface of the crystal, that allowed using the computer program Photoshop CS3 to clearly determine the value of the dislocations' density in the crystal Λ.

According to the Granato-Lucke's [2] theory, in the amplitude-independent area, the dislocation (Λ and L), and the dynamic (B) characteristic for the downstream branch and the resonance region of the curves $\Delta_d(f)$ are tied by the correlations:

$$\Delta_m = 2{,}2\Omega\Delta_0\,\Lambda L^2;\; f_m = \frac{0{,}084\pi C}{2BL^2};\; \Delta_\infty = \frac{4\Omega G b^2 \Lambda}{\pi^2 B f} \quad (3)$$

where Δ_∞ – the value of the decrement for frequencies $f >> f_m$; Ω – the orientation factor, which takes into account that provided reduced shear stress in the slip plane is less than the applied stress; L – average effective length of the dislocation segment; $\Delta_0 = (8\text{Gb}^2)/(\pi^3 C)$, C – effective tension of a curved dislocation ($C = 2\cdot\text{Gb}^2/\pi(1-\nu)$); Λ – the dislocation density; ν – the Poisson's ratio; G – shear module of the active slip systems; b – the magnitude of the Burgers' vector [2].

For all the above ionic crystals, the value of the Debye temperature was determined by performing the calculations according to the Launay's method [3]. The basis for the calculations θ, as well as for $\Omega(T)$, $G(T)$, $C(T)$, $\nu(T)$, $B(T)$ and $L(T)$ were the temperature dependences of the elastic modules $C_{ik}(T)$ of the crystals, which in turn, were based on the data of the temperature dependences' measurements of the longitudinal and transverse ultrasound waves' velocity in the directions of <100>, <110> and <100> respectively. The density of the dislocations was determined independently – by the method of etching pits.

From the correlations (3) it can be vividly seen that, in the presence of data on Λ in unexplored crystals, the method [3] allows not only to reproduce the curve $B(T)$, but also to reveal the frequency spectra family of the dislocation decrement of ultrasonic attenuation in crystals, having corresponding rapper points of resonance and the decaying branches of the curves $\Delta_d(f)$. In addition, the temperature parameter L is clearly established.

That is, we must state that the work [3] gives us the possibilities not only to establish a hierarchy of the existing phonon braking mechanisms of the dislocations in the crystals, but also allows to reproduce the acoustic and structural characteristics of them.

As it is well known, the string dislocation theory [2] operates with two types of pinning centers at dislocations. First, these are the nodes of the dislocation grid (Mott's stoppers) – strong pitch points, the separation of which the model does not allow, and weak blocking centers (Friedel's stoppers) – impurity atoms, pinning centers of radiation and magnetic origin, etc., the rejection of which is possible and is activated, for example, by the magnification of the crystalline temperature, or by an increase in the level of external mechanical stress. Since the frequency spectra of the dislocation decrement of ultrasonic attenuation in crystals are very sensitive [2] to the existing structural defects of the real researched objects, so, they are crucial for all the characteristics that cause the real working of the technique [3], though remained some doubt about its effective application for various objects.

In paper [4], it was shown that the coefficient of dynamic braking of dislocations B, as suggested by the authors [1], is a fundamental characteristic of a crystal that is independent of the investigated object's mechanical state and is determined only by dissipative processes in the phonon subsystem of the crystal. In Fig. 2 one can see that the value of B does not depend either on strong stoppers on dislocations (Λ), or on weak stoppers – defects of radiation origin in a wide range of X-ray irradiation 0-1057 R. Each of the experimental points on straight line 5 is averaging over all values of B, obtained before and after irradiation in the entire range of radiation doses.

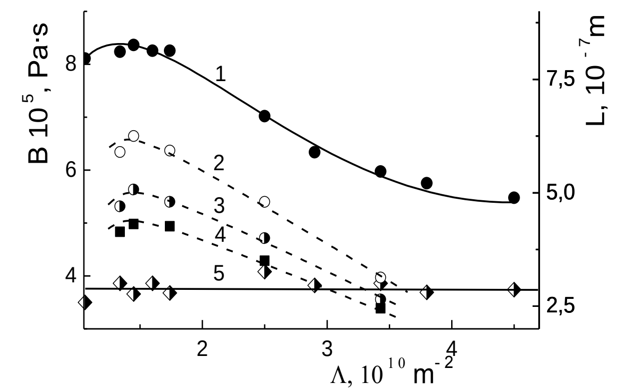

Fig. 2 – Dependences of the parameters L (curves 1-4) and B (5) on the density of dislocations for LiF crystals of different irradiation time t, min: 1 – 0; 2 – 20; 3 – 40; 4 – 60

Fig. 3 demonstrate a qualitatively similar results obtained on the same crystals in another way by studying the dispersion of the ultrasonic waves' velocities in samples.

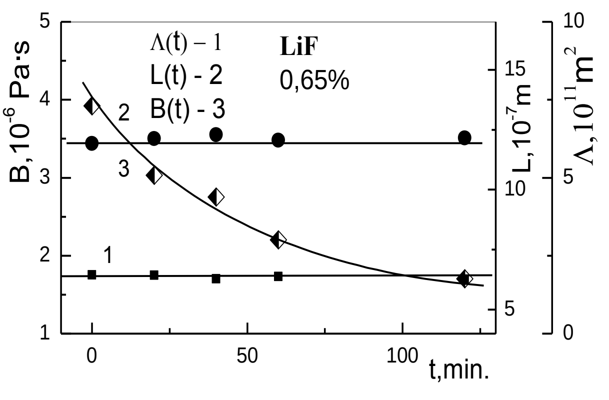

Fig. 3 – Dependence of the density of dislocations (1), the length of the dislocation segment (2) and the coefficient of phonon braking of the dislocations (3) on the time of LiF crystals' irradiation

The above data suggest that the presence of structural defects in crystals does not in any way limit the effectiveness of the method's application [3]. This is clearly illustrated by the independence of the curve $B(T)/B(\theta) - T/\theta$ on the density of dislocations in samples obtained for KBr crystals (see Fig. 4).

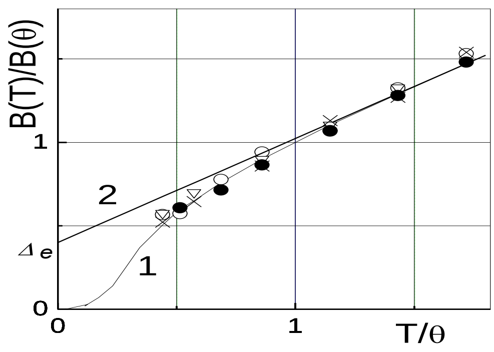

Fig. 4 – Comparison of the combined temperature course $B(T)/B(\theta) - T/\theta$ with experimental data for crystal KBr (o – ε = 0,23 %, ▽, ×, • – data for crystals with deformations ε = 0,5, 0,75 and 1 % respectively); the curve 1 is the Alschyts-Indenbom's theoretical curve calculated according to the experimentally determined phenomenological parameter of the theory Δ_e, line 2 is the high-temperature asymptote through which Δ_e is determined

The paper [5] presents the results of systematic investigations of the radiation defects' nature that arise under the action of X-ray irradiation in the range of doses 0-1057 R. The authors [5] aimed to determine the type of radiation defects, track the dynamics of their formation in irradiated specimens and determine the effect of the samples' dislocation structure on the type and number of radiation defects. For this purpose the authors used the optical absorption method, widely utilized in optical radiation material science, as an instrument for the identification of radiation defects in solids [6-10]. Its essence is to study and analyze the spectral dependences of the transmission coefficient $\tau_\lambda(\lambda)$ for irradiated crystals. In the presence of typical radiation defects, the absorption bands of optical radiation appear on the curves $\tau_\lambda(\lambda)$ in their form and location on the wavelength axis, qualitative and quantitative characteristics of radiation defects can be established. The authors of [5] performed a complex of studies of the dependences on LiF samples that were deformed in the range of 0,155-3,3 % and irradiated to doses in the range of 0-1057 R. The analysis of the curves $\tau_\lambda(\lambda)$ showed that all absorption bands fixed by the authors [5], localized only near $\lambda_{max} \approx 248$ nm, and in other sections $\tau_\lambda(\lambda)$ no else bands were detected. The researches demonstrated that in all studied crystals of lithium fluoride in the range of radiation doses 0-1057 R radiation defects were exclusively F-centers. The possibility of presence in samples F_2-centers ($\lambda_{max} \approx 443$ nm) and F_3-centers ($\lambda_{max} \approx 307$ and 377 nm) the experiment excluded [5]. In order to establish the number of F centers in the samples, the authors [5] used the dispersion ratio of Smakula, which makes it possible to determine the volumetric density of the F-centers of the N_F for the parameters of the absorption band. To do this, the curves $\tau_\lambda(\lambda)$ for crystals with different values of ε were determined by the dependence of the wavelength of the spectral attenuation index $K_\lambda(\lambda)$. Typical $K_\lambda(\lambda)$ dependencies are shown in Fig. 5.

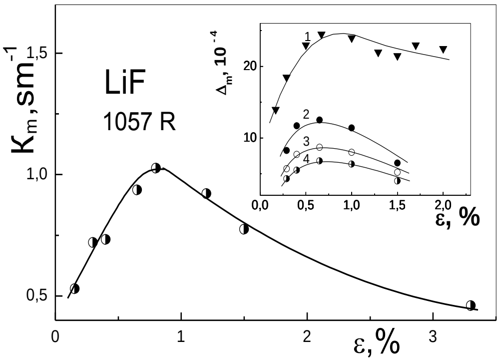

Fig. 5 – Effect of deformation on the spectral index of attenuation in the maximum in LiF crystals

It is clear that dependence $K_m(\varepsilon)$ is non-monotone. At the same time, the maximum of the curve is observed at the area ~ 0,7-0,8 %. From work [4] one can learn that the indicated values of ε for LiF characterize the special state of the deformed crystal, in which dislocations under the action of mechanical stress are maximally detached from their holding stoppers, and the process of their re-attachment, caused by the interaction of the initial dislocations with dislocations of the "forest", has not begun yet. In Fig. 5 for the convenience of comparing the optical and acoustic experimental data, the dependences of the dislocation decreasing decrement of attenuation $\Delta_d(\varepsilon)$ for non-irradiated (1) and irradiated (2-4) LiF crystals are given in the form of an insert. Attention is drawn to the obvious analogy observed in the course of dependencies $K_m(\varepsilon)$ and $\Delta_d(\varepsilon)$. This may indicate that the sound and electromagnetic waves react to the dislocation structure of the crystals in a similar manner, which is quite permissible thing, for the equations of propagation of these waves in the mediums are indeed qualitatively identical. From the results shown in Fig. 5 it follows that the greater is the average effective length of the dislocation segment, the more perceptible are the ultrasonic losses and also the loss of the radiation of the optical range passage through the crystal.

The data, that we obtained in [5] provide a unique opportunity of the transition from acoustic characteristics to optical ones and allow to enhance the technique [3] substantially.

Due to the fact that the optical experiment [5] was carried out on the same irradiated and diffused LiF crystals, as the acoustic studies of dynamic and structural characteristics [4], it is possible to compare the data of the dislocation decrement of ultrasonic attenuation in the maximum with the maximal value of the spectral attenuation index for the crystal.

Accordingly, knowing just two parameters – θ and Λ for any unexplored ionic crystal, one can establish a hierarchy of phonon braking mechanisms of dislocations in a crystal, and can also predict the course of the temperature dependences of the B crystal's dynamic characteristic and structural L, can reproduce the frequency spectra of the dislocation decrement of the ultrasonic attenuation in a crystal and, using the data of Fig. 5, can switch from acoustic to optical characteristics. By reproducing the dependence $K_\lambda(\lambda)$ it is possible to list it in the curve $\tau_\lambda(\lambda)$, which can be directly used for colorimetric studies of the spectrum of radiation passing through the crystal.

Thus, this work gives us rather wide opportunities for future research of ionic crystals, as well as for mutually agreed physical interpretations and comparisons of new findings.

CONCLUSION

1. The factors that influence on the effectiveness of the method in order to predict the level of dislocations' phonon braking in crystals are analyzed in our work. It is vividly shown that structural defects of different physical nature in no way complicate the practical use of this method.

2. For the first time, the capacity of the frequency spectra reproduction of the dislocation absorption in crystals at a known Debye temperature was presented.

3. The possibility of transition from thermal (θ) to structural (Λ, L, N_F), dynamic (B), acoustic (Δ_d), optical (K_m, τ_λ) and colorimetric characteristics was firstly demonstrated. The indicated analytical-calculation algorithms can be useful for the development of elements, devices and systems on their basis.

Емпіричні закономірності змінення з температурою Дебая динамічних, акустичних, структурних, оптичних і колориметричних характеристик іонних кристалів

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У роботі розглянуто можливість встановлення ієрархії фононних механізмів гальмування дислокацій за температурою Дебая досліджуваного кристала. Уперше продемонстровано технологію відтворення частотних спектрів дислокаційного поглинання ультразвуку у кристалах за відомою температурою Дебая, а також показано алгоритм переходу від теплових до структурних, динамічних, акустичних, оптичних і колориметричних характеристик кристалів. Проаналізовано вплив структурних дефектів кристала, зокрема, вузлів дислокаційної сітки і центрів закріплення на дислокаціях різної фізичної природи, на запропоновані емпіричні закономірності і обгрунтовано доцільність їх використання для зразків іонних кристалів з різним механічним станом.

Ключьові слова: Фононне гальмування, Дислокаційний декремент, Деформація, Опромінення, Дислокації, Температура Дебая, Показник ослаблення, Коефіцієнт динамічного гальмування, Пружні модулі.

REFERENCES

1. V.I. Alschits, V.L. Indenbom, *Sov. Phys. Usp.* **18**, 1 (1975).
2. A. Granato, K. Lucke, *J. Appl. Phys.* **27**, 583 (2004).
3. G.A. Petchenko, *Visnyk V.N. Karazin KhNU* **914**, 82 (2010).
4. G.A. Petchenko, *Funct. Mater.* **20**, 315 (2013).
5. G.A. Petchenko, A.M. Petchenko, *Probl. At. Sci. Techn.* **2(96)**, 25 (2015).
6. V.M. Lisitsyn, *Radiation Physics of Solids* (Tomsk: "Tomsk Polytechnic University Publising House": 2008).
7. M.V. Galustashvili, M.G. Abramishvili, D.G. Driaev, V.G. Kvachadze, *Phys. Solid State* **53**, 1412 (2011).
8. V.I. Arbuzov, *Radiation Basics of Optical Materials* (St. Petersburg: "St. Petersburg State University of Information Technologies, Mechanics and Optics": 2008).
9. M.I. Mazuritsky, *X-ray Optics* (Rostov-on-Don: Rostov State University: 2005).
10. I.M. Neklyudov, A.K. Malik, A.A. Parkhomenko, A.V. Rudnitsky, *Probl. At. Sci. Techn.* **93**, 52 (2009).