Formation of Defects by Radiation in KBr-Li and KBr-Na crystals

K.S. Baktybekov, A.K. Dauletbekova

L.N. Gumilyov Eurasian National University, 5 Munaitpassov str., 010008, Astana, the Republic of Kazakhstan, E-mail: mzdorovets@inbox.ru

Abstract – The article regards influence of M_A - impurity (Li^+ and Na^+) on formation of defects by X-radiation in KBr-Li and KBr-Na crystals. The concentration of impurity, temperature of irradiation and dose were determined by the method of absorption spectroscopy. When interaction of moving, non relaxed excitons with the impurity is high (for KBr it is either pre-helium temperature or high-impurity concentration) we can see the picture of suppression by impurity effect of defect of pre-impurity excitation on Frenkel defects in an anion lattice. The dependence of defect-creation for 5K on the concentration of impurity has a linear character. By using this fact the assessment of the exciton's free path yields the 100 lattice constants. Besides we regard a model of tunnel overcharge of F-H_A pair, basing on the F-centre model which supposed that the tunnelling electron is localized on the M_A-ion and if there is an H-centre nearby, so the complex $M^0{}_A Br^-{}_2$ is formed. In the ultimate result the complex turns into I_A–centre.

1. Introduction.

We observe the suppression of radiated defect-formation beginning with just a little concentration of impurity in case of X-irradiation of KBr crystals, containing M_A – impurity (Li^+ or Na^+) for 5K. We discover the same effect for 80K having larger concentration of impurity that is in case when the interaction of exciton with the impurity is high so radiating decay of exciton from ion of impurity would take place without process of defect-formation [1,2,3]. The absorption spectrum of KBr-crystals with M_A– impurity, having X-irradiated at 80K, and depending on level of the concentration of the impurity contain as defects of pure KBr (F, V, α) as impurity radiated defects of interstitial origin: H_A-, I_A-, V_{4A}- centres. Increasing concentration of Na^+-impurity to 1 mol.% we see an effect of moving of radiated defects towards α -I_A pair, we explain it as tunnel overcharge of F-H_A → α -I_A pairs [3]. The view of the absorption spectrum of KBr-Na 1mol.% X-radiated at 80K is simple, they contain absorption bands of α–, F-, H_A- and I_A- centres, but there is no absorption of V-centres.

2. Experimental procedure.

Monocrystals KBr- Li and KBr- Na were grown by Stokbarger's method by means of recourse having cleaned from OH^-. The amount of Na^+-impurity we have defined by the method of spectrum analysis, and concentration Li^+ – by number of impurity radiated defects taking into accountant the saturation of the impurity defects. The results are based on value, assessed by a coefficient of distribution of Li^+ in KBr (0.02–0.03) [4]. The samples were radiated with URS -50 (55 kV, 20 mA, W). The absorption spectra were recorded by means of the Specord UV- VIS.

3. Results and discussion.

We made a graphic of dependence of F- centre absorption on number of impurity ions by means of analysis of absorption spectrum of KBr-LI crystals with different level of the impurity concentration, X-radiated at 5K (Fig. 1).

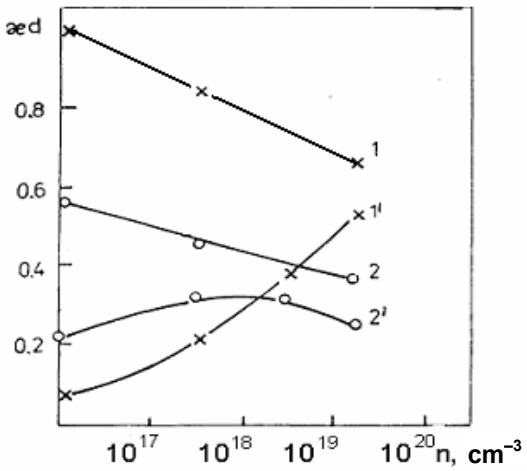

Fig. 1. Dependence of the absorption in I- band at 5.2 eV and in K-band at 2.35 eV on Li^+ concentration for KBr-Li : radiated during 225 minutes for 5 K (1 and 2) and for 80 K (1' and 2')

Taking into accountant the line character of dependence of defect-formation on the impurity concentration we can show the total probability of annihilation of exiton by the formula: $1=P_A+ P_R$, P_A– probability of exciton's autolocalization, P_R– probability of radiated decay of exciton. Less possible canals of annihilation aren't regarded, then:

$$1 - P_A = P_R,\ P_R = R\sigma\ ,\ \text{where}$$

R – the exciton's free path, σ – a section of capture, n-number of impurity ions in 1cm^3, if $\sigma = \pi d^2/4$, d – cation-anion distance, for Li-Br it is $3.17\cdot10^{-10}$m [5] for Rσ we have the value $5\cdot10^{-21}$ cm^3 and for R is

100 lattice constants. So, the exciton's free path in KBr-Li crystals at 5K is about 100 lattice constants.

To demonstrate clearer image of comparison of the dependences we put them onto the same graphic. As it is shown the way of dependence of Li^+ impurity with various temperatures is quite different: the suppression at 5K creation both α – I, and F – H pairs, so the total of vacant defects of $N_{F+}\alpha$ is changed, with increasing to 80 K, by growth of the impurity concentration of $N_{F+}\alpha$ value by comparison with pure KBr. The same you can see for KBr-Na – crystals (Fig. 2).

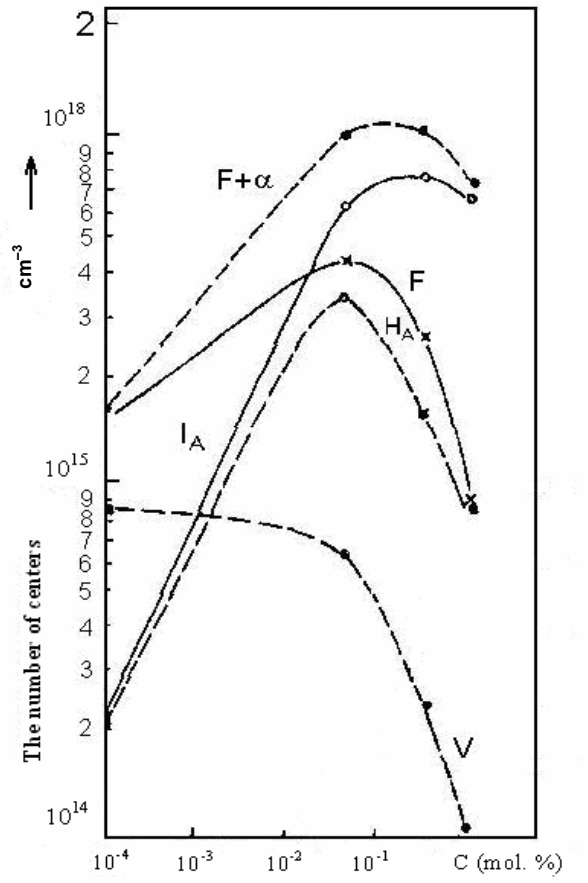

Fig. 2. Dependence of the number of defects (F, H_A, I_A, V and F+α- centers) on Na^+-impurity concentration in KBr-Na : X rayed at 80K for 30 min

Here we have the phenomena of transformation the F – H_A pair into α –I_A pair because of increasing of the M_A – impurity concentration in KBr, that is explained by us as increase of effect of tunnel overcharge of neutral pairs in charged ones [3], there it is given an estimate of the distance in F – H_A pair, when the effect is maximum. The distance is equal to about 2 lattice constants, $(12–15)\cdot10^{-10}$m. With more M_A-impurity concentration when α-band emerged as consequence of α–I pairs absorption, it increases by the same law as F-absorption band (Fig. 3).

It means the transformation leading to creation of stable α–I_A pairs takes place at the distance including thermoactivated move of H-centre. (The transformation F-H_A → α –I_A occurs.)

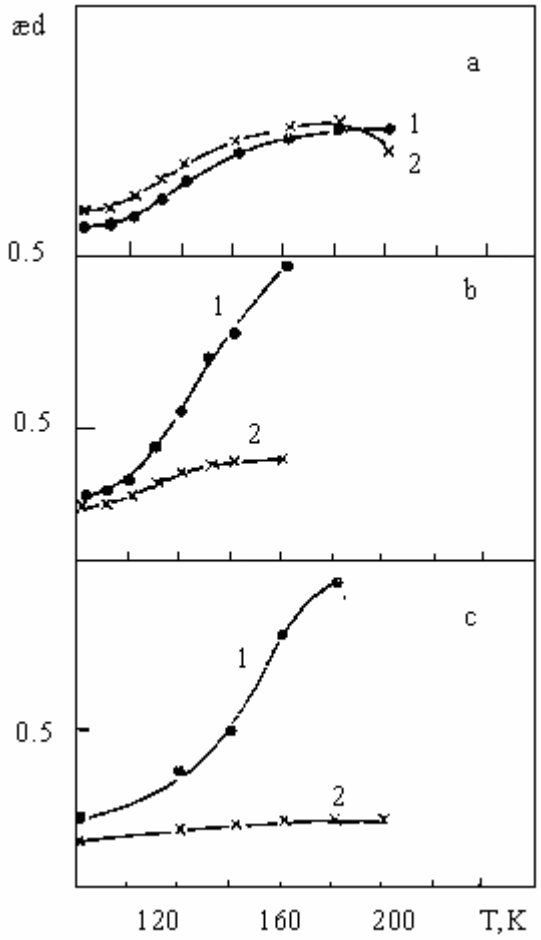

Fig. 3. Temperature dependence of the absorption in α and F- bands (curves 1 and 2) in KBr-Li with concentration of Li 0.2(a), 0.004(b) and 0.0005(c) mol.%. The X- radiation times were the following: 2 min.(a), 5 min.(b) and 15 min. (c)

Now we regard a possible scheme of tunnel overcharge. More tested F-centre is an anion vacancy with localized electron. The electron holds by electrostatic powers. F-centre is paramagnetic centre, its g-factor is almost equal to g-factor of free electron. The sight of the EPR spectrum depends on extra-thin interaction between unpaired F-electron and nucleus, surrounding the anion vacancy with 6 nuclei of the nearest cations. It is shown by the method of double electron-nuclear resonance that the electronic density of F-centre is isotropic and its distribution reminds distribution of electron in an atom of hydrogen in the ground state. Besides it was set up, that about 95% of its time the electron in its ground state is situated in its environs of anion vacancy on the nearest cations and less than 1% on the following cations [6]. With excitation of F-centre the process of F – H_A→ α –I_A transformation accompanying by luminescence with maximum 2.75–

1.80 eV[3]. At this time according to [7] two models of excited F-centre are actively tested: the model of Bogan-Fletcher where for description of the excited state the mixed 2s-2p state is used; the model of Fowler where 2p-like waved function is used. In KBr crystals the analysis of given optical detection of the magnetic resonance shows such part like 2p – state. Therefore, we can say that this excited state is described by 2s-2p functions. As the wave function is more diffusion it is expected the electron of excited F-centre tunnelling may be localized on the impurity M_A -ion, forming a neutral impurity atom, if there is H-centre near, so that we will get molecular formation $Li^0Br_2^-$ or $Na^0Br_2^-$ with further transformation in I_A- centre as a result of transition of the electron to H-centre. The possibility of this transition is regarded in the model of dynamic crowdion. The dynamic crowdion according by [8] is a close-packed anions with an extra ion. We get such row in the localization of electron to H-centre. Emerging unstable state, can turn into stable one by means of displacement of one from ion row to interstitial, the displaced ion is I-centre.

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