The Influence of Low Temperature Uniaxial Stress on Migration and Stabilization of H – Centers in Alkali Halide Crystals

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Abstract – With the methods of absorption, luminescence and thermal activation spectroscopy it has been established that in KBr and KCl crystals at lattice symmetry lowering by low temperature uniaxial stress a stabilization of traveling halogen atoms is realized mainly by V_K – center creation. In KBr and KCl crystals an elastic stress brings to effective radiation conversion of X_3^- – into X_2^- – *centers* at constant concentration of F – centers.

1. Introduction

One of the commonly accepted physical phenomena in alkali halide crystals (AHC) is self – trapped exciton (STE) decay in regular crystal lattice sites into luminescence and initial radiation Frenkel defects. It is known that at non irradiative self – trapped exciton decay in AHC the initial complementary defects are $e_s^0 \to F + H$, where F – center is electron self – trapped in anion vacancy field, thermally stable for all AHC until 400 K, H – center is internodal haloid atom that takes anion lattice site, low temperature radiation defect. That is why the effectiveness mechanism of stable F – center accumulation is conditioned by the stabilization of traveling H – centers, especially at temperatures higher than the delocalization temperature (>55 K). This is proved by the fact that first we observe sharp decrease of F – center concentration in temperature range of H – centers instability and then starting form 80 K – gradual growth to initial level as for the case at 4.2 K. This is conditioned by the realization of different unstable H – center stabilization channels:

$$H\left(X_2^-\right)_a^0 + H\left(X_2^-\right)_a^0 \to \left(X_3^-\right)_{aca}^0 M_i^+ X_i^-, \quad (1)$$

$$H\left(X_2^-\right)_a^0 + H\left(X_2^-\right)_a^0 + \upsilon_a^+ \upsilon_c^- \to \left(X_3^-\right)_{aca}^0, \quad (2)$$

$$H...\left(Na^+\right) \to H_A\left(Na^+\right), \quad (3)$$

$$H + \upsilon_a^+ \to V_K, \quad (4)$$

$$H \to V_K + I, \quad (5)$$

The reaction (1) was experimentally found in and described in details in [1]. The reaction (2) is realized with much probability in plastic stressed crystals when divacancy concentration are specially increased [2]. The reaction (3) is realized with much probability in AHC alloyed with homolog cations of smaller radius than the main cation, for example in KBr – Na.

With the methods of absorption spectroscopy it has been established that in alkali halide crystals at low temperature stress there is conversion of X_3^- – into X_2^- – centers at constant concentration of F – centers. That is why we studies in details the absorption features of halogen centers in AHC at low temperature uniaxial stress.

2. The experimental results

The Figure 1 shows spectra of optic absorption of non stressed (curve 1) and uniaxially stressed (curve 2) KBr and KCl crystals. As it is seen from Figure the nature of appearing radiation defects does not change at stress applying. It is known that in KBr and KCl crystals the main radiation defects are F – and X_3^- – centers. In KBr crystal F – and Br_3^- – centers have absorption bands with maximums at 2.06 and 4.6 eV and in KCl crystal – F – and Cl_3^- – centers – at 2.3 and 5.2 eV respectively (Fig. 1a). In KBr and KCl crystals the concentration of F – centers does not change at stress applying (curves 1 and 2, Fig. 1b). It means there is no change in effectiveness of stable radiation defect creation. Therefore in KBr crystal it has been noticed that there is a redistribution of halogen radiation defects between bands of Br_3^- – and Br_2^- – centers in favor of latter in the range of absorption spectrum that corres – ponds to absorption V_K(3.25 eV), V_{KA}(Na)(3.02 eV), H_A(Na)(3.05 eV) and H(3.26 eV) – centers (Fig. 1a). The found absorption band increase at 3.25eV (Fig. 1c) was thermally annealed at around 200K where V_K(180 K) – centers are troyed. This excludes H_A(Na) – center presence as on spectral content and as on temperature stability. When comparing absorption band spectra maximums of all Br_2^- – center family with absorption band maximum it is seen that at unixial stress there is an increase of concentrations, either V_K(3.25 eV) – , V_F(3.3 eV) – , or H(3.26 eV) – centers (Fig. 1c). It is known that H – centers at KBr crystal ate thermally stable only at 4.2 K and higher 50 K begin to delocalize, and at temperatures where the absorption spectra measurements have taken place (80 K), they are thermally non stable. That is why we think the found absorption band with maximum at 3.25 eV at low temperature stress corresponds to V_K – center, i.e. there is an effect of conversion of H – into V_K – center.

For the experimental disclosure of the effect of V_K – center intensity strengthening we used high sensitive thermal stimulated luminescence (TSL) method; the physical meaning of which is in the registration of recombination luminescence of electron – hole pairs.

As an example Fig. 2 shows the TSL curves, and Fig. 3 – luminescence spectra at optic stimulation and spectra F, F' – KBr crystal luminescence flash. As it is seen from Figure 2 in stressed KBr crystal the TSL intensity peaks V_K (180 K) – , V_F(240 K) – centers increase more than ten times.

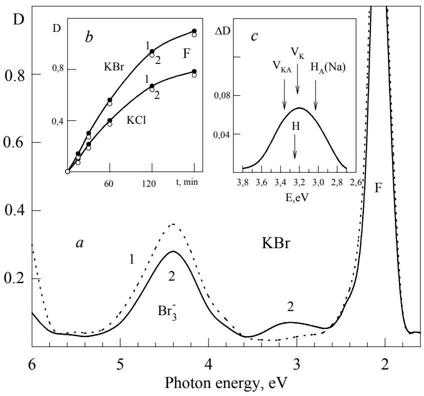

Fig. 1. KBr and KCl crystal absorption spectra:
a – KBr crystal absorption spectra without stress (1) and previously unixially stressed (ε =2%) at 80 K (2) and after X – raying for 3 hours at 80 K; *b* – dose dependences of stable F – center concentration in KBr and KCl crystals before (1) and at uniaxial (ε =2%) stress (2); *c* – deffered KBr crystal absorption spectra before (1) and at uniaxial stress (ε=2%) (2) from graph *a*

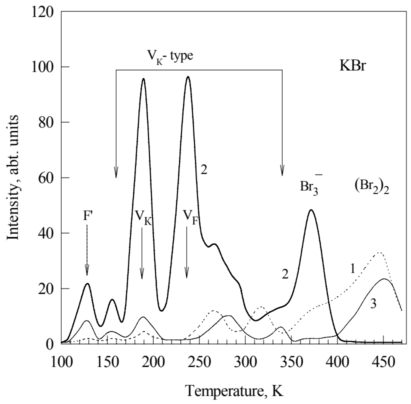

Fig. 2. TSL curves of X – rayed KBr at 80 K in isodosed mode for 1 hour: 1 – not stressed; 2 – stressed (ε =2%) at 80 K; 3 – after heating to 500 K firstly stressed, X – rayed and cooled to 80 K

After mechanical stress removal with heating to 500 K the intensity of V_K – center sharply decreases and becomes comparable with intensity of V_K – center before stress (Fig. 2, curve 3). The same effect of V_K –center ntensity strengthening at lattice symmetry lowering by low temperature stress is found practically for all AHC.

In the field of elastic stress an intensity redistribution of high temperature peaks of thermal stimulated luminescence into low temperature ones, which is conditioned by stabilization of single V_K, V_{KA}, V_F и H_A – centers that belong to family of X_2^- – centers.

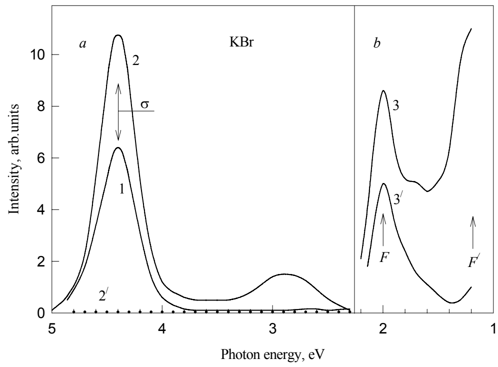

Fig. 3. The luminescence spectra of optic stimulated (a) and F spectra, F' – flashes of stressed (b) (ε=4%) and X – rayed for 2 hours at 80 K KBr: 1 – luminescence spectra at optic stimulation at 80 K in the zone of F – absorption band by photons with energy of 2.0 eV; 2 and 2′ – luminescence spectra at optic stimulation at 80 K in the zone of F – absorption band by photons with energy of 1,2 eV before and after crystal stressing; 3 and 3′ – optic luminescence spectra of σ – luminescence at 80 K and after heating to 140 K

According to reaction (5) besides V_K – center, a traveling halogen ion must be created; and with F – center interaction a free electron must be created. But free electron self – trapping can occur in two ways:

$$e^- + F \to F' \quad (6)$$

$$e^- + e_s^+ \to e_s^0 \Rightarrow h\nu(\sigma,\pi) \quad (7)$$

The similarity of spectrum σ – luminescence of self – trapped exciton and luminescence spectrum (Fig. 3, curve 2) (registered at optic stimulation in spectral zone of F' – center, which was firstly stressed and X – rayed at 80 K) proves experimental disclosure of reaction (7). F, F' – flashes of σ – luminescence of stressed KBr crystal, are thermally destroyed after heating the crystal to 140 K where F' – centers are thermally destroyed. In KBr crystal the luminescence spectrum (Fig. 3, curve 2′) does not exist before stress at optic stimulation in spectral zone of F' – centers.

Abovementioned experimental results on absorption and luminescence spectroscopy are evidence to the fact that lattice symmetry lowering of KBr crystal by low temperature uniaxial stress promotes a stabilization of traveling internodal halogen atom as V_K – center.

References

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