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Mechanisms for Enhancing Luminescence Yield in KBr Crystals under the Influence of Low-Temperature Uniaxial Elastic Deformation

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Abstract: This study investigates the radiative relaxation of electronic excitations through luminescence spectroscopy techniques applied to high-purity KBr crystals subjected to low-temperature (85 K) uniaxial deformation along the $\langle 100 \rangle$ and $\langle 110 \rangle$ crystallographic directions. Results demonstrate that the most significant enhancement in the intensity of σ -(4.42 eV) and π -(2.3 eV) luminescence from self-trapped excitons in KBr crystals occurs with elastic deformation along the $\langle 110 \rangle$ direction, aligning with the axis of the hole component of the anion self-trapped exciton. Deformation-induced changes in X-ray, tunneling, and thermally stimulated luminescence spectra reveal a new band, denoted as E_x , peaking at approximately 3.58 eV, attributed to tunneling charge exchange between the F' - and V_K -centers in their ground state.

Keywords: ionic crystal; high-purity KBr crystal; self-trapped exciton; uniaxial deformation; low temperature; X-ray luminescence; tunnel luminescence; thermally stimulated luminescence



Citation: Shunkeyev, K.; Sagimbayeva, S.; Ubaev, Z.; Kenzhebayeva, A. Mechanisms for Enhancing Luminescence Yield in KBr Crystals under the Influence of Low-Temperature Uniaxial Elastic Deformation. *Crystals* **2024**, *14*, 698. <https://doi.org/10.3390/cryst14080698>

Academic Editors: Xianshao Zou and Wenping Yin

Received: 24 April 2024

Revised: 31 May 2024

Accepted: 6 June 2024

Published: 31 July 2024



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1. Introduction

There has been a renewed focus on investigating the radiative relaxation of electronic excitations (ERs) within ionic crystals (ICs) in recent years. This resurgence is fueled by the promise of new technological applications such as cryodetectors for detecting dark matter [1–3] and nanotubes with hexagonal and octagonal cross-sections [4–7]. These studies aim to provide detailed insights into the intrinsic luminescence and point radiation defects of these crystals [8–10]. Notably, such investigations heavily rely on the use of external factors to disrupt the symmetry of the crystal lattice, that include local deformation caused by the introduction of impurity ions [11–14], as well as thermoelastic [15–17], uniaxial [18–22], and isotropic deformation [23–26]. Of particular interest is the utilization of low temperature uniaxial deformation, which amplifies the likelihood of self-trapping of free excitons at regular lattice sites, leading to characteristic σ - and π -luminescence [20]. This method has proven successful in confirming the intrinsic nature of the E_x -luminescence observed in elastically deformed RbI [27] single crystals.

Nowadays ionic crystals serve as ubiquitous optical materials, exhibiting transparency across a broad spectral range, exemplified by LiF and NaF [8,9]. These materials find extensive application as scintillation materials [28–31], thermoluminescent dosimeters [32–36], and luminophores [37–39] crucial for visualization and detecting ionizing radiation in various fields such as the nuclear industry, medicine (PET and SPECT tomography) [40,41], and ecology [42].

The investigation of electronic excitations' relaxation in the infrared (IR) spectrum under external perturbing factors aims to enhance light output, thus advancing the development of novel scintillation materials with superior luminescent properties [11–14,43,44]. Traditional scintillators, including NaI and CsI single crystals, remain prominent, leveraging energy transfer from the absorbed matrix to impurity luminescence centers via

electron–hole pairs. These scintillators continue to serve as standard detectors of ionizing radiation due to their high light output and find utility in cryodetectors [1–3], as well as in testing modern optoelectronic devices [45,46].

Exploration of nanotubes within the IR spectrum holds significant promise in pioneering new, structurally stable configurations at exceedingly small scales [4–7].

The objective of this investigation is to examine the impact of low-temperature (85 K) uniaxial elastic deformation (applied along the $\langle 100 \rangle$ and $\langle 110 \rangle$) on the luminescence properties of a KBr single crystal. It encompasses the radiative decay of self-trapped excitons (STEs), a form of intrinsic luminescence, as well as tunneling charge exchange occurring within pairs of radiation defects. The research represents a logical extension of our previous inquiries conducted on KCl single crystals subjected to uniaxial deformation [13,14,16,18].

2. Materials and Methods

KBr single crystals utilized in this research exhibit a low concentration of uncontrolled impurities ranging from 0.01 to 1.0 ppm and were grown at the Institute of Physics, University of Tartu (Estonia). The growing process for these ultrapure crystals involved complex purification procedures of raw materials, including drying of powdered raw materials, melt processing in a halogen stream and multiple zone melting during the final stages. Subsequently, single crystal growth was achieved through the Stockbarger method within an evacuated ampoule. Comprehensive details regarding this growth methodology can be found in the prior literature [9,13,14].

Deformation-stimulated luminescence of the crystals was examined in a special cryostat [47], enabling the application of varying degrees of uniaxial deformation along different crystallographic directions ($\langle 100 \rangle$, $\langle 110 \rangle$) at 85 K. Radiation was recorded both during stress application and following its removal from the crystal.

Bremsstrahlung emitted from the RUP-120 X-ray installation equipped with a W-anticathode, operating at 3 mA and 100 kV, served as the ionizing radiation source.

The X-ray luminescence (XRL) and tunnel luminescence (TL) spectra of the crystals within the 6.0–1.5 eV range were meticulously recorded employing a high-aperture MSD-2 monochromator, an H 8259-01 photomultiplier from Hamamatsu, and the specialized SpectraScan program [14,18]. The scanning velocity for X-ray spectra was maintained at 10 nm/s, while for TL and thermally stimulated luminescence (TSL) spectra, it was set at 50 nm/s.

Furthermore, integrated thermally stimulated luminescence (TSL) was recorded by subjecting a pre-irradiated crystal to gradual heating at a constant rate ($\beta = 0.15$ K/s) utilizing an H 8259-01 detector alongside a specially developed ThermoScan program [14,18].

To determine the activation energy E of luminescence quenching, the Mott formula was used:

$$E = \frac{k \left[\ln \left(\frac{I_0}{I_1(T_1)} - 1 \right) - \ln \left(\frac{I_0}{I_2(T_2)} - 1 \right) \right]}{\left[\frac{1000}{T_2} - \frac{1000}{T_1} \right] 10^{-3}}, \quad (1)$$

where k is Boltzmann's constant, I_0 is the luminescence intensity before the start of temperature quenching, and $I_1(T_1)$ and $I_2(T_2)$ are the intensity values at the beginning and end of the luminescence quenching process.

3. Results

3.1. X-ray Luminescence of Crystals KBr for Uniaxial Deformation in Directions $\langle 100 \rangle$ and $\langle 110 \rangle$

In KBr single crystals, one of the intrinsic radiation phenomena is the luminescence of anionic self-trapped excitons (STEs) observed at low temperatures, exhibiting maxima at 4.42 eV (σ -polarized, with a half-width band of 0.34 eV at 4.2 K) and 2.28 eV (π -polarized, with a half-width of 0.67 eV) [8,48]. These luminescences undergo rapid quenching with increasing temperature, evident by an approximately 30-fold decrease in σ -luminescence intensity and a staggering 300-fold decrease in π -luminescence intensity by 80 K. Nevertheless, the utilization of highly sensitive fluorescence equipment enables the recording of

both X-ray bands, serving as reference signals in this study to investigate the deformation effect at 85 K (see Figure 1, curve 1).

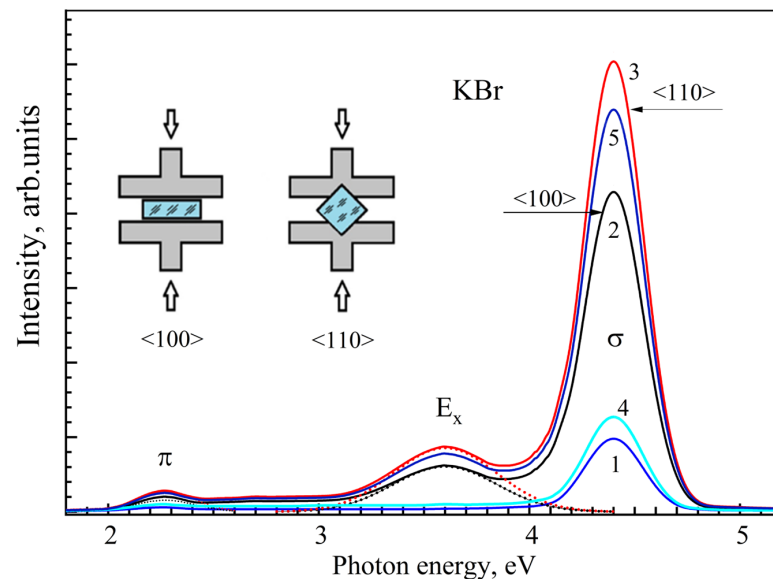


Figure 1. The X-ray spectra of the reference KBr crystal, measured at 85 K prior to deformation (1), during continuous uniaxial deformation ($\varepsilon \approx 1.0\%$) along either the $\langle 100 \rangle$ (2) or $\langle 110 \rangle$ (3) direction, subsequent to removal of the deformation (4), and upon reapplication of the deformation to the initial compression level (5). Dashed lines represent elementary Gaussians obtained by decomposing the X-ray luminescence spectra. The inset schemes illustrate the positioning of the crystals (highlighted in blue) between the clamping cheeks of the cryostat when subjected to uniaxial compression along the $\langle 100 \rangle$ and $\langle 110 \rangle$ directions.

As depicted in the data presented in Figure 1, an increase in the degree of relative uniaxial deformation of the KBr crystal (along $\langle 100 \rangle$ or $\langle 110 \rangle$) correlates with an enhancement in the intensity of both STE luminescence bands. Moreover, an unanticipated X-ray band emerges with a peak at 3.58 eV. The light output enhancement effect of STEs in KBr crystals [18] needs a more detailed investigation taking into account tunneling pairs of radiation defects under the influence of elastic uniaxial deformation.

We denoted this newly identified emission band as E_x , and analogous luminescence is observed in KI and RbI crystals, which also demonstrate sensitivity to elastic uniaxial deformation and are partially associated with a specific STE configuration (i.e., possessing intrinsic characteristics) [27].

It is imperative to underscore that the enhancement in the intensity of all three luminescences at the same degree of uniaxial deformation ($\varepsilon \approx 1.0\%$) is more pronounced when the crystal is compressed along the $\langle 110 \rangle$ direction than in the case of a similar compression along $\langle 100 \rangle$ (compare curves 2 and 3 in Figure 1). The inset in Figure 1 schematically illustrates the crystal's location between the clamping cheeks of the cryostat during the application of uniaxial deformation along the $\langle 100 \rangle$ and $\langle 110 \rangle$ directions. Uniaxial deformation along the $\langle 110 \rangle$ direction was predominantly utilized in this investigation of KBr crystals with a cubic crystal lattice.

The direct correlation between the enhancements of the σ - and π -bands of intrinsic luminescence of STEs with the application of uniaxial deformation to the KBr crystal is further confirmed by the X-ray spectra recorded after the removal of stress and subsequent repeated application at 85 K with the same degree of elastic compression (Figure 1, curves 4 and 5, respectively).

Elastic deformation $\varepsilon \approx 1.0\%$ amplifies the STE luminescence bands by 4–5 times. However, upon removal of compression, an immediate attenuation of approximately 90% in the intensities of σ - and π -emission is observed. Notably, the removal of compression

results in the complete disappearance of the E_x -luminescence, which emerged during deformation with a peak at 3.58 eV (Figure 1, curve 4). Subsequent repeated application of uniaxial deformation at 85 K with the identical ε value (feasible with the cryostat utilized without the necessity for interim depressurization [47]) fully reinstates the intensities of all three X-ray bands observed during the initial compression of the sample (Figure 1, curve 5).

Figure 2 illustrates the dependencies of $I = f(\varepsilon)$, showcasing the intensities of exciton and E_x -luminescence concerning the degree of uniaxial deformation exerted on the KBr crystal along the $\langle 110 \rangle$ directions at 85 K. Analysis reveals that the intensities of σ - and π -luminescence of STEs exhibit a linear increase up to $\varepsilon \approx 1.0\%$, beyond which a saturation stage commences. In contrast, the intensity of E_x -luminescence demonstrates a linear rise up to 2% deformation without any indications of saturation (Figure 2, curve 3). This observation suggests the ongoing accumulation of radiation defects (generated during the measurement of X-ray laser spectra), which contribute to the 3.58 eV luminescence. It is noteworthy to reiterate that the linear segment of the dependence $I = f(\varepsilon)$ for σ - and π -luminescence of STEs corresponds to the elastic part of the uniaxial deformation of the KBr crystal.

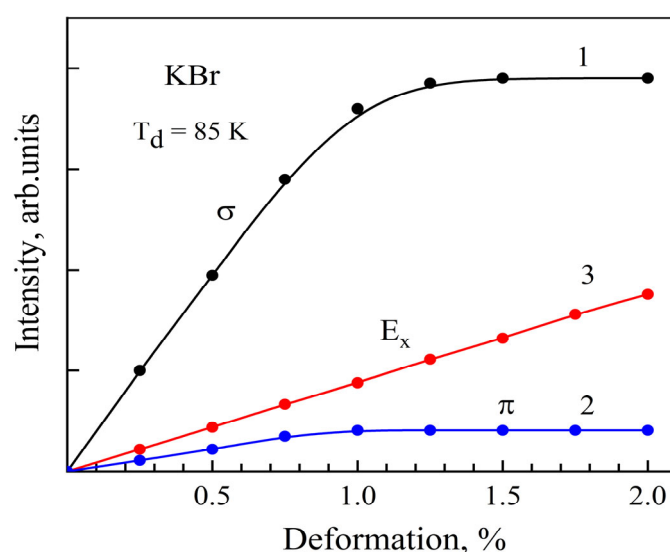


Figure 2. Dependences of the intensity of σ -(1) and π -(2) luminescence of STEs (maxima at 4.4 eV and 2.3 eV, respectively) and E_x -(3) band of the X-ray laser (3.58 eV) on the degree of uniaxial deformation ε by $\langle 110 \rangle$ at 85 K.

Deformation-stimulated enhancement of σ - and E_x -luminescence in KBr is exclusively observed under low-temperature uniaxial compression (85 K) of the crystal. In Figure 3, the temperature dependencies of σ - and E_x -luminescence intensities are depicted in Arrhenius coordinates for the KBr crystal subjected to uniaxial deformation $\varepsilon \approx 1.0\%$ along the $\langle 100 \rangle$ direction at 85 K. These dependencies were recorded by varying the temperature during the acquisition of X-ray spectra in both directions: from low to high (85 $\rightarrow$ 130 K), and from high temperature to lower (130 $\rightarrow$ 85 K). Utilizing the Mott formula (1) (as detailed in Section 2 and [9]), luminescence quenching activation energies of 0.167 eV and 0.2 eV for σ - and E_x -luminescence, respectively, were determined from these temperature dependencies.

In our assessment, the activation energy for quenching σ -luminescence signifies alterations in the temperature-dependent height of the potential barrier between radiative and non-radiative STE annihilation processes. As the temperature rises, the efficiency of radiative decay diminishes (reflected by an increase in the barrier's height). Extinguishing E_x -luminescence aligns with the temperature range of active thermal decomposition of F' -centers (consisting of two electrons trapped in the vicinity of the $v_a^+ e^- e^-$ anion vacancy) within KBr crystals (110 $\div$ 120 K [49]), with the activation energy for quenching this luminescence corresponding to the thermal ionization energy of F' -centers (0.2 eV). Consequently, one of the contributing partners to the recombination process of E_x -luminescence is the F' -center.

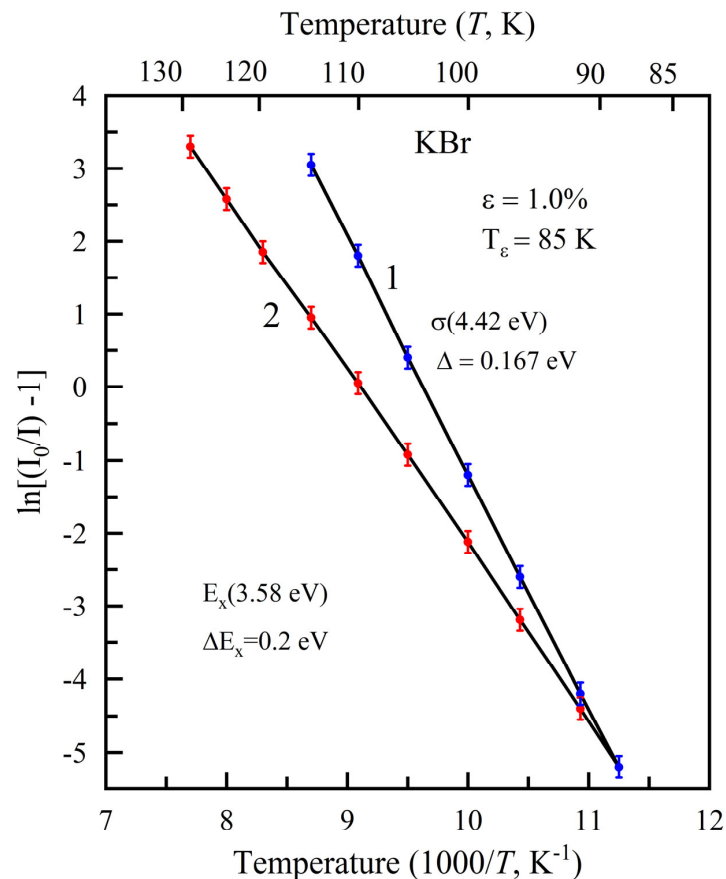


Figure 3. Temperature dependence of the XRL intensity at 4.42 eV (graph 1—STE σ -emission) and 3.58 eV (graph 2— E_x -emission) in Arrhenius coordinates for a KBr crystal under uniaxial deformation applied at 85 K ($\langle 110 \rangle$, $\varepsilon \approx 1.0\%$).

3.2. Tunneling Luminescence of KBr Crystals under Uniaxial Deformation

The 3.58 eV band (E_x -emission), initially identified by us in the X-ray spectrum of a KBr crystal deformed at 85 K, is also evident in the tunnelling luminescence (TL) spectra of crystals subjected to compression conditions during X-ray exposure (Figure 4, curves 2 and 2').

In the temperature range from 4.2 to 77 K, TL in KBr crystals has been extensively investigated and is primarily attributed to tunneling electron–hole recombinations involving F- and V_K -centers in their ground state [50,51]. The F-center, historically the first color center discovered, represents an electron localized in the field of the $v_a^+ e^-$ anion vacancy (for example, see in [8]), while a V_K -center constitutes a self-trapped hole occupying two adjacent anion sites of a two-halide quasimolecule (in KBr, this is $(Br_2^-)_{aa}^+$) [9,52].

It can be suggested that the E_x -(3.58 eV) luminescence detected in the X-ray spectra of KBr crystals elastically deformed at 85 K also possesses a tunneling nature. In the TL spectrum of an X-rayed KBr crystal, the E_x -band predominates and is described by a Gaussian curve (dashed curve 2' in Figure 4) with a half-width of 0.5 ± 0.05 eV. Note that in X-rayed but undeformed KBr crystals, this luminescence could not be registered in the TL spectrum at 85 K, presumably due to insufficient concentration of F'- and V_K -centers (Figure 4, curve 1).

In high-purity KBr crystals with minimal concentrations of impurity ions (0.01–1.0 ppm), the range of radiation defects potentially contributing to TL is restricted to several anion and cation Frenkel defects—F-, $(Br_3^-)_{aca}$ -, F'-, and V_K -centers [8,9,49,50,52–54]. The $(Br_3^-)_{aca}$ -center represents a trihalide quasimolecule localized within two anion and one cation lattice sites. It is essential to consider F'- and V_K -centers as plausible tunneling pairs for TL formation with a peak at 3.58 eV.

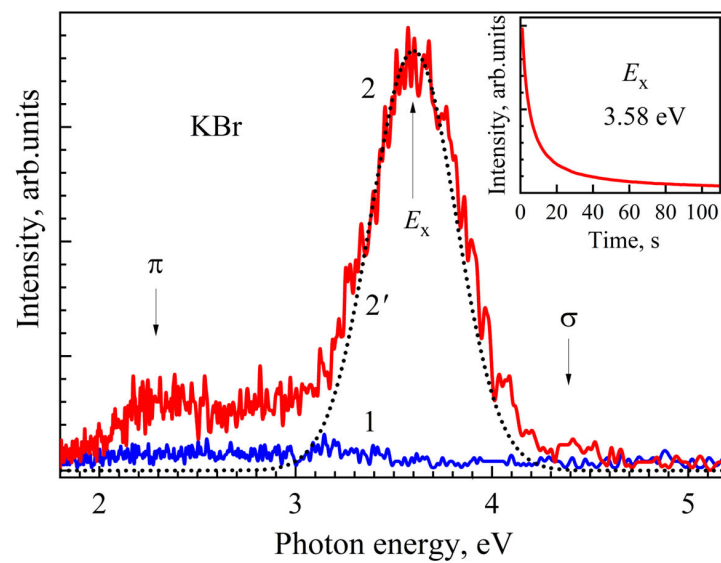


Figure 4. The TL spectra of a KBr crystal recorded at 85 K subsequent to isodose irradiation with X-rays (W-anticathode, 120 kV, 5 mA, 30 min, 85 K). Curve (1) represents the TL spectrum in the absence of deformation, and curve (2) represents the TL spectrum under the influence of uniaxial deformation ($\epsilon \approx 1.0\%$, $\langle 110 \rangle$). The elementary Gaussian (2') characterizing the TL spectrum is shown. Additionally, the inset illustrates the attenuation of E_x -TL at 85 K in a deformed KBr crystal.

From the quenching curve of tunnel E_x -luminescence provided in the inset of Figure 4, it can be inferred that in the deformed lattice of KBr, electron–hole tunneling recombination in pairs of spatially close defects, most likely F' - and V_K -centers, ceases by 25–30 s, while pairs of spatially separated defects continue to contribute to TL up to 100 s.

Drawing parallels with the scenario involving Tl_0 - V_K and Ag_0 - V_K pairs in doped KCl crystals [55], we examined the possibility of a tunneling electronic transition between the primary levels of F' - and V_K -centers in KBr crystals subjected to uniaxial compression at 85 K (see Figure 5 and Table 1).

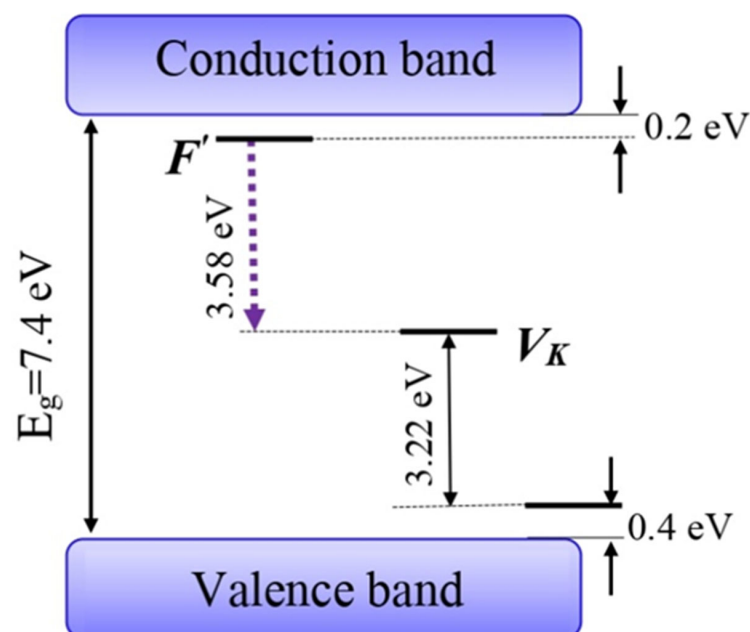


Figure 5. Simplified energy diagram illustrating the nature of E_x -(3.58 eV) luminescence during a tunneling electronic transition between the main levels of F' - and V_K -centers in KBr crystals subjected to uniaxial deformation at 85 K.

Table 1. Optical characteristics [8,9,56] of KBr and KCl crystals. E_g is a band gap for KBr and KCl crystals at 80 K.

Crystals	E_g (eV)	Maximum Optical Absorption V_K -Center (eV)	Thermal Dissociation Energy V_K -Center (eV)	Thermal Dissociation Energy F' -Center (eV)	Maximum E _x -Tunnel Luminescence (F' -, V_K -Centers) (eV)
KBr	7.4	3.22	0.4	0.2	3.58 ¹
KCl	8.5	3.4	0.54	0.3	4.26 ²

¹ Experimentally established spectral region of tunnel luminescence (F' -, V_K -centers) in KBr based on materials from this publication (see also Figure 5). ² Estimated spectral region of tunnel luminescence (F' -, V_K -centers) in KCl.

The band gap in KBr is $E_g = 7.4$ eV [8–10]. The optical transition in the V_K -center corresponds to an absorption band peaking at 3.22 eV, and the activation energy (0.4 eV) characterizing the delocalization of the V_K -center enables the determination of the main level's position relative to the top of the valence band (3.62 eV) [56].

Therefore, considering the band at 3.58 eV of TL originating from the ground level of the F' -center, the latter should trail the bottom of the conduction band by approximately 0.2 eV. This value coincides closely with the activation energy for the thermal destruction of F' -centers documented in the literature [49].

Hence, as per the illustrated band diagram, a tunneling electronic transition between the ground states of the F' - and V_K -centers in elastically deformed KBr crystals, culminating in the emission of a luminescence quantum at 3.58 eV (indicated by the purple dotted line in Figure 5), has been convincingly established.

Based on the optical characteristics for KCl crystals, a prediction of spectral region for the tunneling charge exchange of F' - and V_K -centers with a peak at approximately 4.3 eV has been documented similarly (Table 1).

3.3. Thermally Stimulated Luminescence of KBr Crystals under Uniaxial Deformation

As highlighted in the previous section, the influence of elastic deformation prompts the appearance of a TL signal in KBr at 3.58 eV, indicating an increase in the concentration of F' - and V_K -centers. Consequently, this development offers the prospect of detecting these defects by observing characteristic TSL peaks attributed to the delocalization temperature of the F' - and V_K -centers (125 K and 165 K, respectively [9,56]).

Figure 6 illustrates the integrated TSL curves for KBr crystals, recorded during pre-isodose heating X-rayed at 85 K in the absence of deformation (curve 1) and at elastic compression applied at 85 K (curve 2).

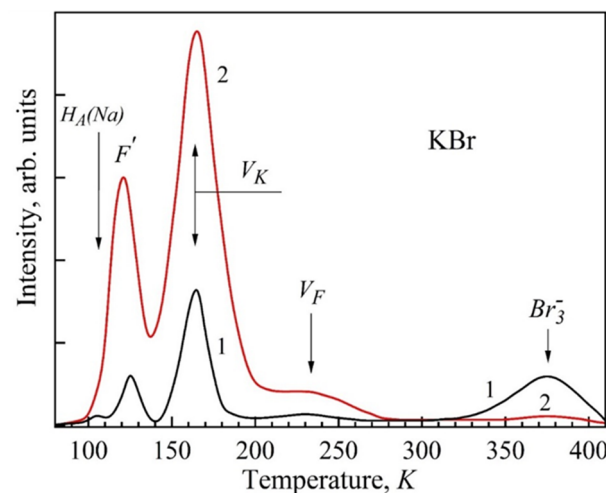
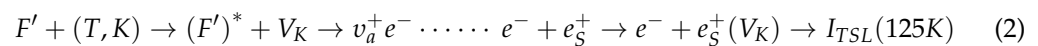


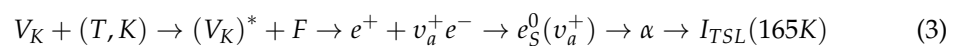
Figure 6. Integral TSL of KBr crystal, isodose-irradiated with X-rays (W-anticathode, 120 kV, 3 mA, 85 K, 60 min) 1—in the absence, 2—under the influence of uniaxial deformation ($\epsilon \approx 1.0\%$, $\langle 110 \rangle$). Linear heating rate $\beta = 0.15$ K/s.

A comparison of curves 1 and 2 in Figure 6 reveals that the application of elastic uniaxial deformation stimulates the generation of intrinsic radiation defects, leading to pronounced low-temperature TSL peaks at temperatures of 125 K (F'-centers) and 165 K (V_K-centers). It is worth noting that, in the absence of deformation, weak TSL peaks associated with complementary F-type Frenkel defects (of the vacancy type) to interstitial halogen ions/atoms are observed at temperatures below the delocalization temperature of F'-centers [9,10]. Additionally, within the depicted temperature range in Figure 6, TSL peaks corresponding to interstitial ions and halogen atoms localized in the field of uncontrolled impurity sodium ions are visible [13,14] (I_A(Na) and H_A(Na), respectively). Annealing of I_A(Na)- and H_A(Na)-centers occurs almost simultaneously, posing a challenge for their differentiation based on temperature (refer also to [14]).

In a deformed crystal, these TSL peaks are significantly suppressed. During thermal ionization of F'-($v_a^+ e^- e^-$) centers at about 125 K, the released electron (e^-) has a high likelihood of undergoing radiative recombination with a self-trapped hole, i.e., a V_K-center according to the following scheme:

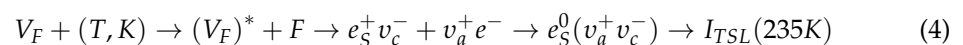


A similar process occurs during thermal delocalization of V_K-centers. In this case, a mobile hole (e^+) recombines with an electron of the F-($v_a^+ e^-$) center, thermally stable up to significantly higher temperatures (~400 K) [9,52–54]:



According to scheme (3), during recombination of the mobile hole with the F-center an exciton-like formation similar to an α -center with a characteristic emission is created in the field of an $e_S^0(v_a^+)$ anion vacancy [9,10,53,57].

At 235 K, a TSL peak was recorded (more pronounced in a deformed crystal) associated with the delocalization of the V_F-hole center, a self-trapped hole in the field of a cation vacancy ($e_S^+ v_c^-$) [9,10]. The registration of this peak in a deformed KBr crystal is facilitated by a high concentration of cation vacancies created by deformation (v_c^-):



A mobile V_F-center, formed after localization of a V_K-center nearby, according to scheme (3), interacts with the F-center and creates an exciton-like formation in the $e_S^0(v_a^+ v_c^-)$ divacancy field [13,14,53,57], the radiative decay of which gives the emission at 235 K.

Hence, in an elastically deformed KBr crystal, robust TSL peaks attributed to F'-(125 K) and V_K-(165 K) centers were detected. Meanwhile, a TSL peak at 380 K associated with the thermal destruction of trihalide quasimolecules Br_3^- , formed through the paired interaction of interstitial halogen atoms [9,13,14,52–54], experienced notable suppression. The elastic deformation of the KBr crystal impeded the migration of interstitial halogen atoms throughout the crystal lattice, thereby facilitating their conversion into V_K-centers and the accumulation of F-centers to maintain the electrical neutrality of the crystal lattice.

Indeed, the findings from TSL measurements indicate that sustained elastic uniaxial deformation effectively fosters the formation of F'- and V_K-centers in KBr crystals (compare curves 1 and 2 in Figure 6).

This circumstance prompted us to study the TSL spectra (Figure 7) of deformed KBr crystals with the anticipation of unveiling the spectral composition of the supposed interaction products presented in schemes (2', 3', 4').

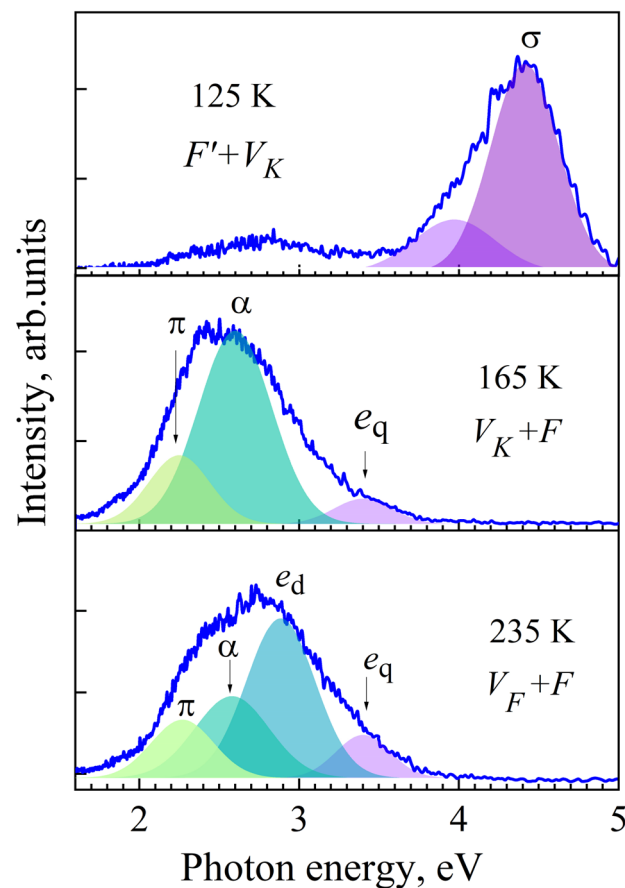
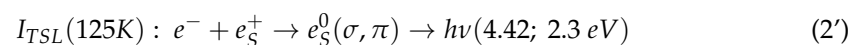


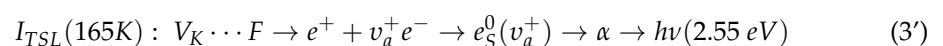
Figure 7. Spectra of TSL peaks at temperatures of 125 K, 165 K, 235 K, and 380 K of a zone-purified KBr crystal under direct influence of uniaxial deformation ($\varepsilon \approx 1.0\%$, $\langle 110 \rangle$, 85 K), after irradiation with X-rays for 1 h at 85 K (W-anti-cathode, 120 kV, 3 mA, 85 K). Arrows indicate the spectral positions of the present emission bands in the form of Gaussians. Colors are selected in accordance with the corresponding spectral regions of the electromagnetic wave scale.

The dominant TSL spectrum at 125 K corresponds to the σ -luminescence emission band (4.42 eV), as a result of the recombination of free electrons (e^-) with self-trapped holes (e_S^+), creating a formation similar to a self-trapped exciton $e_S^0(\sigma, \pi)$:



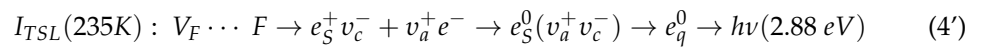
It should be noted that π -luminescence (2.3 eV) practically does not appear in the TSL spectra, apparently due to significant temperature quenching compared to σ -luminescence (4.42 eV). According to data [48], their intensity differs by almost 100 times.

In the temperature range corresponding to the thermal delocalization (165 K) of V_K -center holes in the TSL spectra (curve 2 of Figure 7), luminescence arising from the recombination of mobile holes with electron radiation defects, $F(v_a^+e^-)$ -centers, is observed:



As a result, an exciton-like formation is generated, perturbed by anion vacancy $e_S^0(v_a^+)$, the so-called α -luminescence, which has a maximum at 2.55 eV. In the TSL spectra at 165 K, a non-elementary emission band was detected in the spectral region at $2.4 \div 2.6$ eV.

When $V_F(e^+v_c^-)$ -centers interact with $F(v_a^+e^-)$ -centers, the environment of the formed exciton-like formation will be disturbed by a divacancy $e_S^0(v_a^+v_c^-)$, according to data [57], which has a maximum at 2.88 eV and is denoted (e_q^0):



In the TSL spectra at 235 K, luminescence was recorded, the maximum of which occurred in the region of 2.8 eV due to the perturbation factor from α -(2.55 eV) and π -(2.3 eV) luminescence (curve 3 in Figure 7).

Thus, by simultaneously recording the integral and spectral thermally stimulated luminescence of KBr crystals under the influence of low-temperature (85 K) uniaxial deformation ($\varepsilon \approx 1.0\%$), the following were established: firstly, the dynamics of growth in the efficiency of low-temperature radiation defects in F' -, V_K -, and V_F -center formation, and secondly, the spectral composition of recombination luminescence products during thermal delocalization of F' -, V_K -, and V_F -centers.

Generally, high-temperature peaks of TSL IR [58,59] form the basis of thermally stimulated dosimetry, the essence of which is that the number of emitted quanta (light yield) during heating is directly proportional to the dose of ionizing radiation received by the sample in a certain period of time.

4. Conclusions

In high-purity KBr single crystals subjected to uniaxial deformation at 85 K, a notable increase is observed in both the intrinsic luminescence of STEs (σ - and π -luminescence) and the E_x -luminescence at 3.58 eV, associated with tunneling charge exchange of F' - and V_K -centers in the ground state.

The X-ray luminescence yield amplifies as the degree of uniaxial compression increases up to approximately $\varepsilon \approx 1.0\%$ of the elasticity threshold. In the transition zone towards plastic deformation, a saturation of luminescence intensities becomes apparent with further increments in ε . Of particular note is more pronounced enhancing of luminescence due to elastic compression along $\langle 110 \rangle$ compared to the same deformation along $\langle 100 \rangle$.

A diagram of the symmetric configuration of STEs (type I according to the Kan'no classification [60]), wherein the σ -component of luminescence is distinctly registered during radiative decay, is presented in Figure 8.

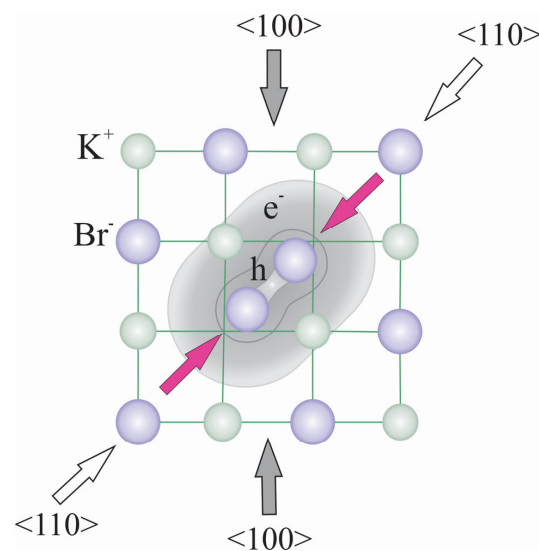


Figure 8. Model representation of the effect of uniaxial deformation in the $\langle 110 \rangle$ and $\langle 100 \rangle$ directions in the KBr crystal lattice, taking into account the STE structure [8,60]. The outer arrows of the figure indicate the directions of uniaxial compression carried out using a special cryostat [47]. Inner pink arrows indicate the directions of anion sliding during uniaxial deformation.

During low-temperature deformation along the $\langle 100 \rangle$ axis from the crystal's end face, the lattice compression occurs effectively along the $\langle 110 \rangle$ direction, aligning with the hole component orientation of the STEs in KBr. In other words, external mechanical tension applies along the $\langle 100 \rangle$ crystal axis, while optimal lattice compression and the best sliding will occur along the STE axis (refer to Figure 7). If the external mechanical tension aligns along the $\langle 110 \rangle$ axis, coinciding with the STE axes in the regular lattice or an exciton-like formation in the field of cationic impurities, one can expect the maximum enhancement effect of luminescence at low-temperature uniaxial deformation of alkali halide crystal under such conditions.

Author Contributions: Conceptualization, K.S.; methodology, K.S. and Z.U.; software, S.S. and Z.U.; validation, K.S.; formal analysis, S.S.; investigation, K.S. and Z.U.; resources, K.S.; data curation, S.S.; writing—original draft preparation, K.S.; writing—review and editing, A.K.; visualization, S.S.; supervision, S.S. and A.K.; project administration, K.S.; funding acquisition, K.S. All authors have read and agreed to the published version of the manuscript.

Funding: The research was conducted as part of a grant project funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23488688).

Informed Consent Statement: Informed consent was obtained from all subjects involved in the study.

Data Availability Statement: The original contributions presented in the study are included in the article; further inquiries can be directed to the corresponding author/s.

Acknowledgments: The authors express their sincere gratitude to A. Lushchik for stimulating discussions and A. Tilep for depicting TSL spectra graphs, as well as the team of Zhubunov University and the scientific center “Radiation Physics of Materials” for support in fundamental research and discussion of the results obtained.

Conflicts of Interest: The authors declare no conflicts of interest.

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