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Computer Simulations of I-Center Annealing in KCl and KBr Crystals

Theoretical Interpretation of Thermostimulated Experiments

By

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Results of computer simulations of the kinetics of correlated annealing of pairs of close α -I and F-I centers in KCl and KBr crystals, enhanced by I-center diffusion and Coulomb or elastic attractions, respectively, are presented. Special attention is paid to the conditions under which multi-stage annealing stages arise as it has been observed experimentally more than once. Our general conclusions are: (i) a weak elastic interaction affects the recombination kinetics and the survival probability even for relatively well-separated F-I pairs, the more so is true for the case of Coulomb attraction between charged α -I pairs; (ii) the multi-step (kink) structure arises only for close (typically, up to fourth-nearest neighbour) defects. To explain the strongly separated stages observed experimentally for α -I (17 to 21 K, 30 to 39 K in KCl and 18 to 22 K and 27 to 30 K in KBr) a very particular initial distribution of defects is required consisting of two groups of close and well-separated defects. It gives strong support to the results of recent computer simulations that an interstitial ion created due to electron trapping by an H center can be transformed into a crowdion which could be displaced athermally by a long distance from a vacancy (five to seven interionic distances).

1. Introduction

Low-temperature ionizing irradiation of alkali halide crystals produces various types of defects. It is now well-established that primary defects, formed via the nonradiative decay of self-trapped excitons, are Frenkel pairs consisting of neutral $F(v_a^+ e^-)$ and $H(i_a^- = X_2^-)$ centers [1, 2] which are spatially well correlated. Besides, charged Frenkel defects, i.e. empty anion vacancy (v_a^+) and interstitial anion (i_a^-), called α and I centers, are also observed [3]. After prolonged irradiation their concentration could be quite high, e.g. in KBr crystals irradiated at 10 K the ratio of the number of α -I Frenkel pairs to the number of F-H pairs may be about four or five [4].

Frenkel defect annealing is caused by I and H center motion when the temperature increases, since their electron partners (α and F centers) become mobile at much higher temperatures, close to or higher than RT. Their recombination with electron centers leads to the release of stored energy in the form of heat [5 to 8] or luminescence (TSL) [9 to 20],

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and is associated with several decay stages of lattice parameter/crystal volume as a function of temperature [3, 6 to 8, 21], as well as with the appearance of a set of other thermally-stimulated kink dependencies, such as current (TSC), depolarization current (TSDC), and emission-desorption of halogen atoms [9, 11, 16].

In recent years, a complex of optical, structural, and electrical investigations of defect-induced processes observed during thermal annealing of Frenkel defects in alkali halides were performed in a number of research laboratories over the world which allowed to clarify in more detail the mechanisms of their radiation damage and annealing. In particular, the annealing kinetics of primary Frenkel defects – F, H centers in KBr and KCl – crystals were discussed by us in recent papers [22, 23]. Now we focus on the annealing kinetics of *secondary* radiation defects.

The purpose of this paper is, first of all, to review and discuss briefly what is known about the recombination kinetics of I centers in KCl and KBr crystals. The I centers are the most mobile radiation-induced defects in ionic solids and thus necessarily contribute to several kinds of low-temperature diffusion-controlled processes to be discussed in Section 2. In Section 3 we have calculations of the relevant diffusion-controlled processes incorporating I-center diffusion, elastic or Coulomb interaction with F and α centers, respectively, and their annihilation when defects are approaching each other within a clear-cut instability radius. Section 4 summarizes the results of our study.

2. Mechanisms of I-Center Formation and Recombination

First, let us summarize briefly the possible mechanisms of I-center production.

(i) A hypothesis of the $\alpha(v_a^+)$ and $I(i_a^-)$ center creation in a *primary* radiation-induced process of self-trapped exciton (STE) decay was considered in [9, 12]. This is a modification of the original excitonic model by Pooley [24] who was the first to suggest that nonradiative recombination of e^- with a V_K center (self-trapped hole, STH) leads to the dissociation of V_K centers and the ejection of halogen ion (X^-) from a regular lattice site into a tetrahedral interstitial position, i.e.



(ii) Another idea of the direct α, I pair creation as a result of hole trapping by F centers and/or electron trapping by H centers was presented and discussed in [25, 26]:

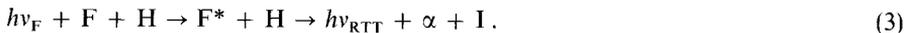


(iii) α, I -center formation can take place via the STE decay into close F–H pairs accompanied by the subsequent *secondary* reaction of the electron tunneling transfer between F and H centers through the reaction [9]



which is a nonradiative process.

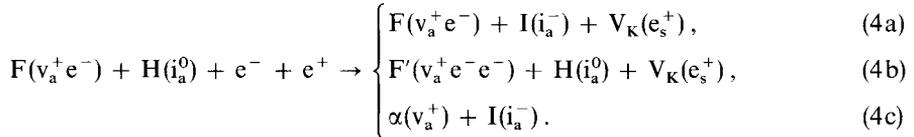
Thus, the tunneling charge transfer, when it is *photostimulated* into the F absorption band, leads also to the formation of α –I pairs through the reaction [15, 16, 19]



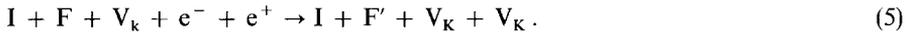
Quantum mechanical cluster calculations [27] have shown that direct F–H tunneling recombination is a nonradiative process whereas its photostimulation (3) is accompanied

by the emission of a photon with the energy distinctive for the so-called “radiative tunneling transition” (RTT). Its theoretical estimate (≈ 3 eV in KCl) was confirmed later experimentally [28].

(iv) A further careful analysis of the different thermostimulated processes studied by means of EPR of hole centers has led to the hypothesis about the formation of *triplets* and *quartets* of Frenkel defects (for details, see [16]). The basic idea is that primary F–H pairs could interact with radiation-induced electron and hole pairs, which may result in the following processes [9, 16, 19]:



According to the numerous experimental data, the creation of the $\{F-I-V_K\}$ *triplet* via the reaction (4a) is predominant in KCl and KBr crystals [9, 16, 17, 19]. The formation of defect quartets was also suggested in [16] as



It should be stressed here that it was just the idea of defect triplets which allows one to interpret in a noncontradictory way a large quantity of experimental data, in particular, the simultaneous observation of STE luminescence, TSC, and TSDC [9, 16].

The important question arises which kinds of spatial defect distributions could be expected from these mechanisms of I-center creation? Since the probability of the tunneling transfer of an electron inside the electron–hole (called also donor–acceptor) pair depends *exponentially* on the relative distance between defects, it is easy to estimate [23, 27] that in the steady-state experiments the separation between α –I partners should not exceed the third neighbours along the $\langle 110 \rangle$ axis. This is in agreement with recent ODEPR low-temperature studies [29], molecular dynamics simulations [30], and the theory of the temperature dependence of F center accumulation in alkali halides [31]. However, it can happen that electron trapping by H centers can result in crowdion formation. Computer simulations of this process [30] have shown that as a result an interstitial halide ion, i_a^- , could be displaced *athermally* by a rather long distance from a vacancy. In the experimental studies on KCl [19, 32] it was suggested to range up to seven interatomic spacings. This could be true for both equation (2) and (4a) and (4c). Therefore, one can expect a *broad* distribution function within F, I and α , I pairs consisting of a group of closely-spaced defects and well-separated (almost randomly distributed) defects.

Let us discuss now in more detail the relevant experimental data for the two basic ionic crystals KBr and KCl, for which most of the experimental information is available.

2.1 KBr crystals

Annealing of I centers in KBr crystals was experimentally studied more than once (see [32] and references therein). Firstly, their recombination with α centers only has been considered using optical measurements [33]. Four distinctive annealing stages were reported at 11, 17, 19, and 21 K. The first three stages were attributed to first-order reactions whereas the fourth stage fits better to the second-order kinetics. The appropriate activation energies for these annealing stages were found to be about 0.015, 0.03, 0.04, and 0.06 eV, respectively.

Therefore, the activation energy of 0.06 eV was interpreted as the migration energy of a *free* I center (Br^- interstitial ion).

A little bit earlier, Kurz and Gebhardt [34] have studied simultaneous annealing of the α band and of that with absorption at 5.4 eV (which they ascribed to I centers). Only two correlated annealing stages were observed: at 12 and 20 K. As it was said before, the first stage corresponds to the first-order reaction with the activation energy of ≈ 0.04 eV. Another well-pronounced stage of I annealing was also reported in [34] at 25 to 30 K where α annealing is less obvious. Later, the thermally stimulated conductivity (TSC) of KBr crystals irradiated at 10 K was investigated by Taylor [35]; two TSC peaks were observed. The averaged activation energy values are 0.050 eV for the 24 K peak and 0.062 eV for the 27 K peak, respectively. Fuchs and Taylor [36] studied the annealing behavior of KBr by means of simultaneous measurements of TSC and TSL. Over the investigated temperature range (10 to 35 K) conductivity and luminescence behave very similarly, and the luminescence does not change its spectral distribution. Four peaks at 14, 17, 20, and 24 K with the characteristic activation energies ranging between 0.025 and 0.0588 eV were reported. The most prominent peak appears at 27 K. As was shown, it is complex and is characterized by activation energies varying with the increase of temperature between 0.062 and 0.1 eV. The former process has a "mixed-order" kinetics, i.e. there is an excess of recombination centers. At higher irradiation doses this process becomes predominant.

Obviously, the observation of the TSL and TSC practically in the same temperature interval where α [33, 34] and I bands [34] are annealed puts under question the simple α -I recombination model suggested by Itoh et al. [33], since it cannot explain the creation of free electrons resulting in the STE luminescence. As it has been said, the most prominent TSL peak was observed at 27 K and is accompanied with the TSC. Using the polarized luminescence method, it has been shown that the glow peak (or at least, its major part) arises from the recombination of free electrons with self-trapped holes (V_K centers). According to Aboltin et al. [9], free electrons are created due to the reaction between migrating I centers with F centers, that is electrons are released from F centers as a result of the F-I recombination. The released electrons are trapped by V_K centers thus giving rise to the STE. As it was noted by Itoh et al. [13], such an interpretation is in somewhat poor coincidence with the fact that the motion of I centers is initiated around 22 K, according to [33] and [34]. We would like to note here that as follows from [34], the I band is completely annealed above 30 K, i.e. the low-temperature stages at 12 and 20 K could arise either due to motion or rotation of other defects, or due to the I centers interacting with F centers [37]. Note also that the 12 K stage corresponds to the H-center rotation observed at 13 to 16 K [13]. The complex H, V_K , and F annealing stages observed at 12 to 15 K may be attributed (as was done before [33] in explaining the temperature dependence of the F-H tunneling luminescence intensity) to the thermally-activated reorientation of H centers [17]. It was assumed that the rotation of H centers brings them into the instability region where they recombine with the nearest F centers. Since this stage is absent at low doses, these are F centers believed to be from *adjacent* F-H pairs, not from genetically-related pairs.

2.2 KCl crystals

Experimental information on KCl crystals is much less detailed than that known for KBr crystals which has just been discussed above. The α luminescence (which is excited in the α -absorption band and characterizes their concentration) is annealed in the three main

Table 1

Theoretical and experimental activation energies E_a for hops of interstitial halide ions (I centers) in KCl and KBr crystals

direction	KCl		KBr	
	theory	expt.	theory	expt.
[100]	1.89 [39]		2.21 [39]	
[111]	0.44 [39]	0.08 [9]	0.19 [39]	0.05 [9]
[111]	0.28 [40]	0.09 [42]	0.24 [40]	0.06 [33]
[111]	0.13 [41]		0.11 [41]	

stages: at 22 K (I), 30 K (II), and 39 K (III) in KCl, whereas *two* main stages at 20.5 K (I) and 28 K (II) are observed in KBr [14]. These data correlate well with the α -absorption [38] and the stored energy [7] annealing measurements in X-irradiated crystals. The high-temperature stage (III) corresponds to the annihilation of α and I centers which are spatially uncorrelated, including their secondary reactions. The luminescence efficiency per I center destroyed in stage (III) is two orders of magnitude greater than for stages (I) and (II) [14]. In this temperature range, TSL peaks are observed at 39 K in KCl and at 28 K in KBr [14].

A theoretical treatment of Frenkel defect recombination requires the knowledge of the activation energies for the diffusion of I centers which are summarized in Table 1. Obviously, the so-called *interstitialcy* mechanism has the lower energy, this means that in the saddle point the interstitial ion and a regular lattice ion form a dumbbell configuration oriented along the $\langle 111 \rangle$ axis and centered on a regular lattice site. However, theoretical values are very much dispersed, and for the activation energies of *free* I centers in KCl and KBr crystals we used the experimental values of 0.08 and 0.06 eV as the most reliable ones.

3. Results of Theoretical Simulations

The theory of diffusion-controlled correlated annealing of pairs of Frenkel defects was described by us earlier [22, 23]. It should be only noted here that we incorporate the elastic and Coulomb interactions of close defects. The former is characterized by the interaction energy $\varphi(r) = -\alpha/r^3$ [43], where α is the interaction constant and r the distance between the defects. We have found earlier that $\alpha \approx 4 \times 10^{-3}$ eV nm³ for F, I pairs in both KCl and KBr crystals [37]. This is by 30% greater than the value of this parameter for F, H pairs. Some preliminary results for F, I annealing in KBr were presented by us earlier [37] where the I center was assumed to lie at the cube center. However, as follows from the double-force tensor analysis of I centers in KBr [44], it is more likely to form a split interstitial along the $\langle 100 \rangle$ axis. This is why in this paper we assume I centers to be situated in the middle of the Me-X distance rather than in the cube center. The annihilation radius of the mobile I center with α (F) center is close to the interionic distance $r_0 = 0.3$ nm [22], the pre-exponential factor D_0 entering the diffusion coefficient $D = D_0 \exp(-E_a/k_B T)$ is not known very well and we fitted it to reproduce correctly the temperature of the experimentally observed lowest-temperature I-annealing stages, thus getting $D_0(\text{KBr}) = 8 \times 10^9 \text{ nm}^2 \text{ s}^{-1}$ and $D_0(\text{KCl}) = 8 \times 10^{12} \text{ nm}^2 \text{ s}^{-1}$.

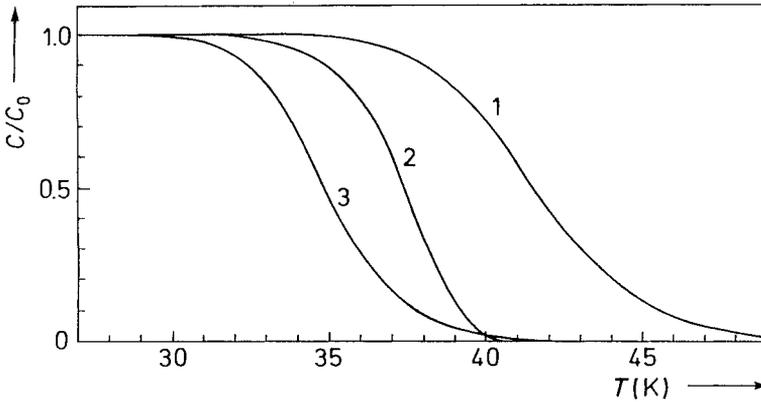


Fig. 1. Uncorrelated annealing of I centers in KCl for the different initial concentrations of defects (in cm^{-3}): (1) $C_0(\text{I}) = 10^{16}$, $C_0(\text{F}) = 10^{16}$; (2) $C_0(\text{I}) = 10^{15}$, $C_0(\text{F}) = 10^{17}$; (3) $C_0(\text{I}) = 10^{18}$, $C_0(\text{F}) = 10^{18}$. Heating rate $\beta = 0.1 \text{ K/s}$

We have simulated below annealing of both, closely spaced and randomly distributed F–I centers. In this section only the results for KCl are presented, whereas the insignificant difference found for the KBr crystals is discussed in Section 4.

In the latter case of uncorrelated recombination defect concentrations obey the ordinary second-order law,

$$\frac{dC_I}{dt} = \frac{dC_F}{dt} = -KC_I C_F, \tag{6}$$

where the reaction rate $K = 4\pi D_I r_0$ and the elastic interaction is no longer important due to a large separation of the defects. As follows from Fig. 1, the distinctive annealing temperature for the free I centers depends considerably on their initial concentration C_0 . It is varying from 30 up to 38 K as C_0 decreases from 10^{18} to 10^{16} cm^{-3} .

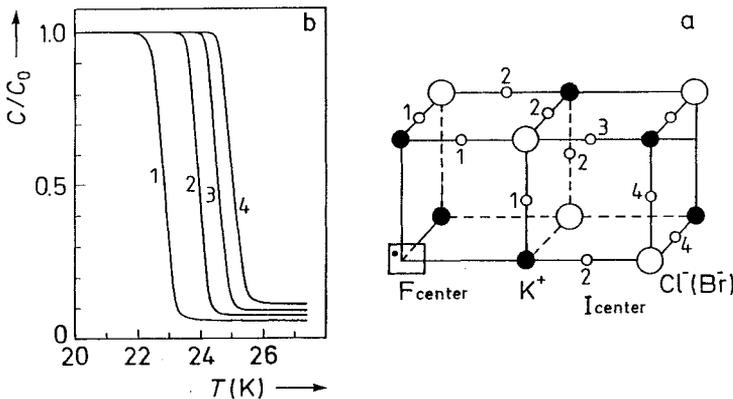
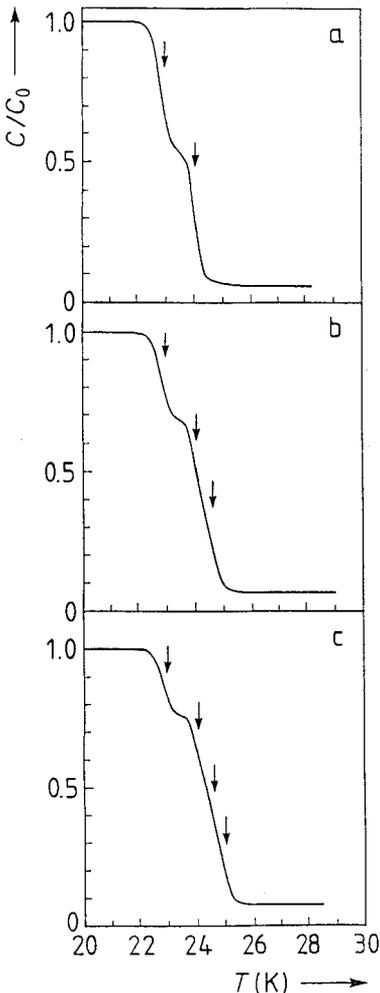


Fig. 2. a) Spatial positions of several types of nearest-neighbor I centers (marked 1 to 4) with respect to the F center put into the coordinate origin. b) The calculated correlated annealing of these close F–I centers in KCl, as controlled by I-center diffusion and the elastic attraction to F center

The results of our calculations for *correlated pairs* are plotted in Fig. 2 to 4. The configuration of several kinds of I centers closely correlated with F centers is shown in Fig. 2a, whereas the calculated decay of their concentrations is plotted in Fig. 2b.

Fig. 2b confirms our previous conclusion [37] that an increase in the distance l between F-I centers from the nearest-neighbour distance (NN) to 4 NN leads to an increase of the annealing temperature. The difference is about 1 K for 1 NN and 2 NN but only 0.5 K for 3 NN and 4 NN. The larger the distance between the defects, the higher is the "survival" probability P_s of I centers (i.e. probability to leave its "own" F center during I-center random walks). For all F-I pairs $P_s \approx 0.08$ to 0.12, i.e. only about 10% of so close defects will participate in the further bimolecular stage of recombination.

The effect of the *simultaneous* annealing of several kinds of defects, which is closer to the experimental situation, is demonstrated in Fig. 3. The conclusion suggests itself that well pronounced steps (kinks) in the I-concentration decay take place only for F-I defects which are separated not further than 3 NN.



The position of a plateau between the first and other kinks is in good agreement with the partial concentration of given I centers. In Fig. 3 it changes from $C/C_0 = 0.5$ (a) to 0.75 (c). The temperature of the beginning of the plateau (23 K) does not depend on the number of NN defects involved. It should be stressed that if we neglected the elastic interaction between the defects, the kink resolution would be considerably worse [22, 23]. The reason of smoothing the stages corresponding to 3 NN and more distant pairs physically is quite clear: the *relative* distance between them in the crystalline lattice becomes less and less; e.g. it decreases from 0.34 for 1 NN and 2 NN down to 0.14 for 3 NN and 4 NN.

Fig. 3. The kinetics of simultaneous annealing of several kinds of NN, F, and I defects in KCl present in equal concentrations. a) 1 NN + 2 NN, b) 1 NN + 2 NN + 3 NN, c) 1 NN + 2 NN + 3 NN + 4 NN. The arrows show the step temperatures for the individual defects, as shown in Fig. 2b. I-center positions are given in Fig. 2a

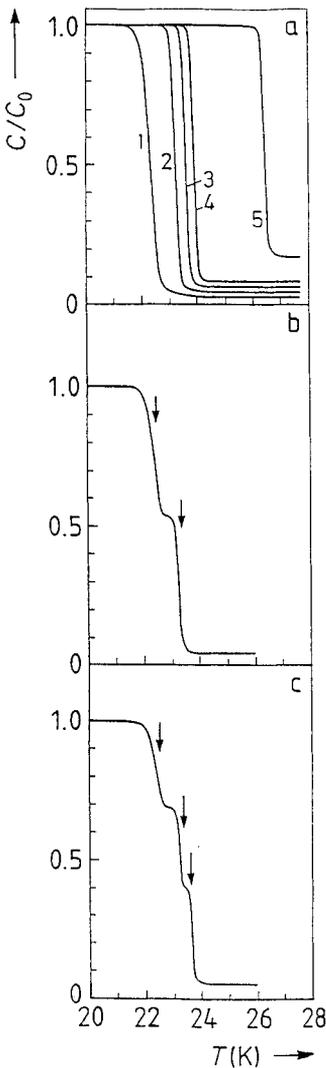


Fig. 4. The kinetics of a) individual and b), c) simultaneous annealing of several kinds of NN, α , I defects in KCl present in equal concentrations. a) 1 NN, 2 NN, 3 NN, and 4 NN (curves 1 to 4, respectively). Curve 5 corresponds to well-separated defects (the distance between α , I centers is 2.33 nm, i.e. they are the 5th neighbors along the $\langle 110 \rangle$ axis). b) 1 NN + 2 NN, c) 1 NN + 2 NN + 3 NN

Lastly, Fig. 4 shows the results for the calculated annealing of oppositely charged defects, i.e. α , I centers. The effect of the strong Coulomb attraction makes steps very sharp and deep. The survival probability of the four types of nearest NN is very small. It increases up to the moderate value of $P_s \approx 0.2$ only for very well-separated defects, 5 NN along the $\langle 110 \rangle$ axis, to be discussed in the following section. The steps are better pronounced here than for the elastic attraction (F-I pairs), but also become closer and closer with an increase of the degree of neighborhood.

4. Conclusions

As follows from our calculations, for F, I spatially-correlated centers the recovery stages at 22, 23, and 24 K in KCl (Fig. 2b) are expected to arise due to very close (1 NN–3 NN) pairs. However, experimental data [32, 43] argue that the relevant temperatures are much higher, 30 to 32 K. This means that in the case of KCl the mean distance between F and I centers (unlike KBr [37]) greatly exceeds that for calculated 1 NN–4 NN. In KBr we observed good agreement between theoretical and experimental stages at 20, 21, and 22 K and 20, 22, and 24 K, respectively [37].

For the pairs of oppositely charged defects, α , I centers, we ascribe the experimentally observed low-temperature recovery stages at 17 to 21 K in KCl [21, 32] and 18 to 22 K in KBr [16, 33, 34] to arise due to similar strongly correlated 1 to 3 NN. In contrast, higher-temperature extended stages (at 30 to 39 K in KCl [14, 20, 21, 32] and 27 to 30 K in KBr [9, 14, 16, 17]) could arise only from *much more* separated defects. Curve 5 in Fig. 4 shows that the stage of α -center annealing at 27 K in KCl corresponds to α -I pairs which are not closer than 5 NN along the $\langle 110 \rangle$ axis. This gives another confidence to the theoretical calculations [30] showing that an athermal crowdion produced as a result of electron trapping by an H center could be displaced by a rather long distance from its vacancy.

Therefore, the experimentally observed low-temperature stages of I-center annealing could be well described using a simple diffusion-controlled model of *interacting* closely-spaced

defects. This interaction makes the step(kink) structure in the annealing curves to be better pronounced. On the other hand, the higher-temperature stages in α -I annealing (30 to 39 K in KCl and 27 to 30 K KBr) seem to arise due to another group of *well-separated* I centers arising as a result of the crowdion ($H + e^-$) formation and its distant athermal motion [30]. Such stages are not observed in F-I recombination, probably because the mobile I centers recombine predominantly with α centers due to their strong Coulomb attraction. It should be stressed here that as it was demonstrated by us earlier, the kinetics of the correlated (geminate) Frenkel defect annealing could be very poorly approximated by the standard first-order rate equations. The more correct formalism requires the use of the diffusion equations which we used here, as well as in [22, 23].

Lastly, simulations of the *free* I-center annealing demonstrates clearly a shift of the recovery temperature with the change of initial defect concentration (i.e. irradiation dose), an effect observed experimentally more than once [20].

In conclusion we would like to stress that the problem of the annealing of spatially correlated Frenkel defects is very universal and actual not only for ionic solids but also for rare gas solids [45], semiconductors [46, 47], and metals [48 to 50]. We believe that for these materials the use of the correct formalism presented by us in [22, 23] and applied here for KCl, KBr crystals could give more quantitative information about the first stages of their radiation damage.

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