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# The mechanism of interaction of dislocations with point defects in ionic crystals

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## Abstract

A mechanism of interaction of dislocations with point defects is suggested on the basis of a study of deformation-stimulated luminescence (DL) from irradiated KCl. DL is considered to be a result of destruction of hole colour centres by dislocations. The centres destroyed by dislocations are responsible for irradiation-induced strengthening of alkali halides.

## 1. Introduction

The problem of how point obstacles are surmounted by dislocations is one of the key issues in the physics of plasticity. In crystalline solids, the initial stress of plastic flow depends on the point obstacles to dislocations. The evolution of the dislocation structure is also largely determined by these defects. However, the experimental methods adopted in the physics of plasticity provide insufficient basis for construction of a microscopic model of interaction between dislocations and point obstacles. Because of this circumstance, an attempt to apply a technique used in another field of physics seems quite reasonable when we try to solve the problem.

Suitable objects for such a study are alkali halide crystals, traditional in solid-state physics. The point obstacles can be produced in them through addition of impurities or by exposure to ionizing radiation. In the case of the irradiation-induced strengthening, the part of the obstacles is played by colour centres. The colour centres are electronic excitations that may relax through interaction with moving dislocations. Deformation-stimulated luminescence (DL) demonstrates that the relaxation does occur. It is well known that DL accompanies plastic deformation of irradiated alkali halides and originates from destruction of some colour centres by dislocations (this destruction gives rise to movable species which recombine radiatively with localized centres) [1, 2].

It is quite possible that dislocations destroy colour centres that are obstacles to them; if so, detection of DL may prove to be a suitable technique for studying the influence of point defects on the dislocation motion. This method could crack one of the central experimental problems,

which arises from the fact that the behaviour of alkali halides upon plastic deformation is largely determined by the interaction between dislocations themselves [3]. As a result, it is very difficult to gauge the contribution of point obstacles against this background. At the same time, the DL is a direct response of the crystal to interaction of dislocations with nothing but the radiation-induced point defects.

Until recently, there have been no reliable data concerning the structure of colour centres acting as obstacles to dislocations, the same being true for centres destroyed by dislocations. The authors of [2] suggested that dislocations destroy hole-type centres, which gives rise to mobile interstitials. In most studies, however, dislocations are believed to destroy electron-type centres, which in the first place refers to F centres (see a review in [4]). This opinion is mostly based on the fact that deformation lowers the concentration of F centres [4]; however, these data are insufficient for reaching a definite conclusion, since destruction of hole-type centres is also accompanied by the disappearance of F centres (colour centres disappear in pairs through recombination).

As to the nature of irradiation-induced strengthening, F centres and vacancies are known to be weak obstacles to dislocations. By contrast, hole centres strongly hinder dislocation slip. It has been shown [5] that interstitial halide atoms and ions (H and I centres, respectively) are principal irradiation-induced obstacles at low temperatures. H and I centres become mobile and vanish in pure alkali halides below liquid-nitrogen temperature. At this and higher temperatures, strengthening is ascribed to  $V_K$  and  $V_F$  centres [6] which become unstable below room temperature (RT). The nature of irradiation-induced strengthening of alkali halides at RT remains unclear. It has been noted [7] that strengthening may be caused by  $V_2$  and  $V_3$  centres, but their structure remains unknown up to now.

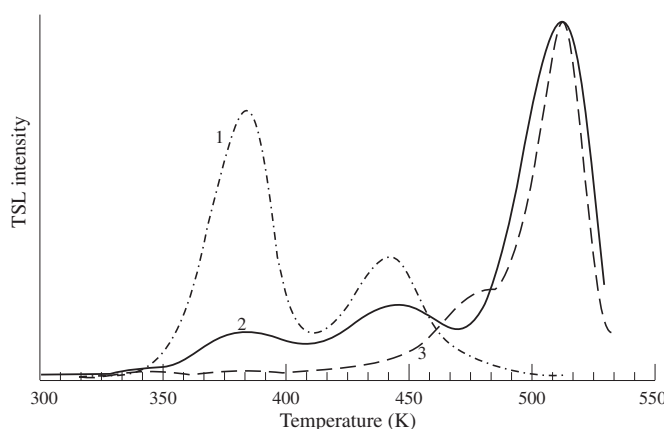
The aforesaid suggests that DL may be a very promising tool for investigating motion of dislocations, provided, however, that it is studied more thoroughly.

## 2. Experimental details

We used nominally pure single crystals of KCl as the objects of study. The crystals were  $\gamma$ -irradiated at RT, using  $^{60}\text{Co}$  as a source, to an absorbed dose of 2 MGy. When samples irradiated to a dose of 0.1 Gy were required, x-irradiated crystals were used. After irradiation, the crystals were cleaved to give samples with dimensions  $5 \times 2 \times 2$  mm. The composition and concentration of the electron-type colour centres were determined from the absorption spectra of the crystals. The concentration of F centres reached  $5 \times 10^{18} \text{ cm}^{-3}$  in the  $\gamma$ -irradiated crystals, and was less than  $10^{16} \text{ cm}^{-3}$  in those irradiated with x-rays. The information on the hole-type centres was obtained from an analysis of glow curves of thermally stimulated luminescence (TSL). The glow curves were recorded in the range 300–550 K with temperature elevated at a rate of  $0.1 \text{ K s}^{-1}$ . The luminescence was detected using a photomultiplier tube incorporated into a single-particle counting system and sensitive to light over the wavelength range 200–800 nm. When studying DL, the load on a sample was recorded simultaneously with the luminescence intensity. Samples were deformed at RT at a rate  $5 \times 10^{-4} \text{ s}^{-1}$ .

## 3. Results

The glow curves for KCl samples are shown in figure 1. A KCl sample irradiated to a dose of 0.1 Gy exhibits two glow peaks at 380 and 450 K (line 1). These peaks are attributed to, respectively, decay of  $V_Z$  and  $V_2$  centres [8, 9]. Deformation of such a sample is accompanied by a DL similar to that described in the literature [4, 10]. It may be concluded that the DL



**Figure 1.** Glow curves for KCl. Samples irradiated to a dose of 0.1 Gy (curve 1) and 2 MGy (curve 2); a sample irradiated to a dose of 2 MGy and annealed at 445 K for 30 min (curve 3).

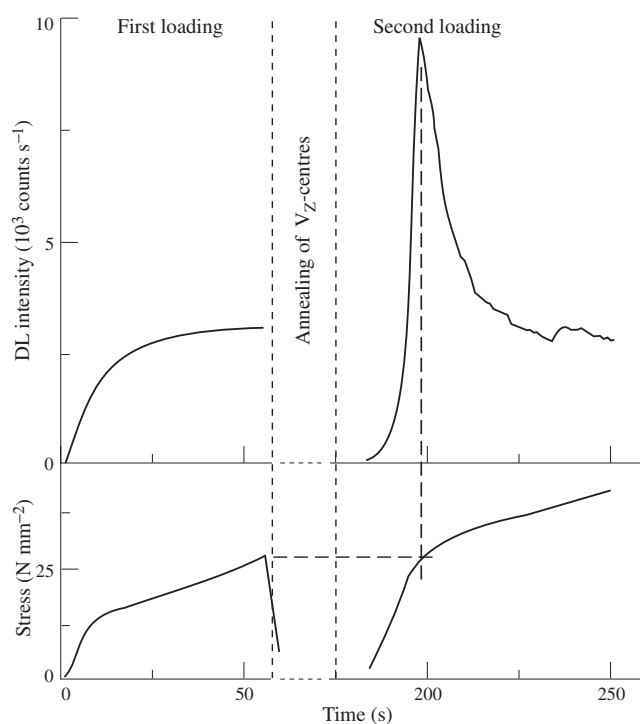
results from dislocation-related destruction of either F-type centres (F, F<sub>2</sub>, and F<sub>3</sub>) or V<sub>Z</sub> and V<sub>2</sub> centres, since glow curves and absorption spectra demonstrate that the concentration of other centres in the samples is negligible. Obviously, the nature of the centres destroyed by dislocations can be established in experiments with crystals containing different sets of colour centres. Since F-type colour centres are always present in radiation-coloured pure alkali halides, samples with and without V<sub>2</sub> and V<sub>Z</sub> centres could be tested. However, such experiments cannot be carried out with the samples described above, since destruction of V<sub>Z</sub> and V<sub>2</sub> centres results in complete decoloration of the crystals (this is a consequence of the fact that V<sub>Z</sub> and V<sub>2</sub> centres are the only hole-type centres in the samples).

With the aim of preparing coloured samples without V<sub>Z</sub> and V<sub>2</sub> centres, heavily irradiated KCl crystals were examined. It has been suggested [11] that intensive irradiation produces some unknown hole-type centres in KCl. This can be seen from the glow curve for a sample irradiated to a dose of 2 MGy, shown by curve 2 in figure 1. In addition to the two peaks that we are familiar with, the glow curve has an intense peak at 515 K. The structure of the colour centres responsible for this peak remains unknown. It has also been suggested that dislocations are structural elements that are necessary for these colour centres to exist [11]. The suggestion is based on the fact that the peak at 515 K arises when

- (i) hard irradiation generates dislocation loops in a crystal or
- (ii) a crystal is deformed prior to being irradiated (in this case, a heavy irradiation dose is not required).

It should be noted here that, in numerous studies, dislocations have been considered likely traps for interstitials; e.g., calculations demonstrate [12] that coupling of two H centres near a dislocation can give rise to a colour centre stable at RT.

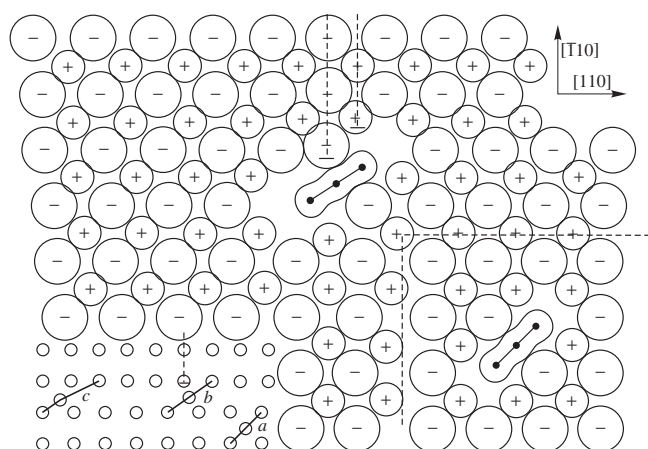
The assumption that the centres are localized at dislocations is supported by the following experiments. An irradiated (2 MGy) sample of KCl was strained at RT to ~2%; the DL intensity was  $\sim 3 \times 10^3$  counts s<sup>-1</sup> (figure 2, first loading). After stress removal, the sample was heated to 370 K, i.e., to the temperature of V<sub>Z</sub>-centre decomposition. Mobile species formed in the process (H and V<sub>F</sub> centres [8]) recombine with F centres or, provided that the assumption mentioned above is correct, give rise to new colour centres as a result of their trapping by strain-induced dislocations. It is important that these dislocations are mobile, as opposed to radiation-induced dislocation loops. Then the sample was allowed to cool, and, thereafter, the



**Figure 2.** DL of a KCl sample loaded in two runs. After the first loading the sample is unloaded, heated to 370 K, allowed to cool to RT, and, thereafter, the interrupted deformation is continued (second loading).

interrupted deformation was continued, again at RT. The results we obtained are presented in figure 2 (second loading). The stress–strain curve shown in the figure can be divided, as is usually done, into two parts: the quasi-elastic and deformation-induced hardening stages. On reloading, the quasi-elastic stage lasts until the stress in the sample exceeds that reached during the preceding load. At this stage, a dislocation does not move as a whole, but its fragments are shifted somewhat: dislocation segments bend between obstacles pinning the dislocation. In familiar experiments with reloading, no DL is detected at this stage, since the dislocation segments move over the area that they have already swept during the preceding run, leaving no colour centres to be destroyed (for details, see [4]). By contrast, we could observe DL at this stage in our experiment, with intensity considerably higher than that recorded during the first loading. By the end of the quasi-elastic stage, the DL intensity reaches its maximum and then decreases to the magnitude recorded during the first loading and retains this value during the stage of deformation-induced hardening. The rise in DL at the quasi-elastic stage of reloading could be attributed, in our opinion, to interstitials trapped at dislocations during the sample heating. As the dislocation segments shift, they move away from these interstitials, which leads to detrapping of the species and, consequently, to luminescence.

As the heavily irradiated crystals of KCl accumulate the colour centres associated with the glow peak at 515 K, they can be used to prepare coloured samples containing no  $V_Z$  or  $V_2$  centres. For this purpose, an irradiated crystal should be either stored at RT in the dark for a sufficiently long period of time [13], or heated to a temperature at which  $V_2$  centres are destroyed.



**Figure 3.** KCl crystal with  $X_3^-$  centres: the (001) plane perpendicular to the edge dislocation with a Burgers vector along the  $[110]$  direction.

Curve 3 in figure 1 is the glow curve of a sample annealed at 445 K for 30 min. The peaks at 380 and 450 K disappear upon annealing, and a vague peak at 470 K, related to  $V_3$  centres [8], becomes visible. The peak at 515 K remains virtually unchanged. The concentration of F centres decreases upon annealing by no more than 10%.

During deformation of unannealed samples, the DL was similar to that shown in figure 2 (first loading), with the DL intensity of approximately  $3000 \text{ counts s}^{-1}$ . The deformation of annealed samples was also accompanied by DL, but the DL intensity was, in this case, only  $200 \text{ counts s}^{-1}$ , i.e., an order of magnitude smaller than that recorded prior to destruction of  $V_Z$  and  $V_2$  centres.

#### 4. Discussion

The above experiment shows that the RT DL of KCl crystals is due to  $V_Z$  and  $V_2$  centres, while the F-type centres play only a secondary role in this process, contrary to common opinion. Dislocations appear to destroy  $V_Z$  and  $V_2$  centres—with  $V_F$  and H centres formed as a result. These centres are mobile at RT, so they recombine with localized F-type centres, which gives rise to luminescence. In order to understand how dislocations can destroy hole centres, we should consider the process of their interaction on the microscopic level.

The  $V_2$  centre is a linear molecule of the  $X_3^-$  type (trihalide molecule) [8] oriented along the  $\langle 100 \rangle$  directions, occupying two anion and one cation lattice sites; the same molecule is incorporated into the  $V_Z$  centre. In the case of KCl, this is the  $\text{Cl}_3^-$  molecule. Figure 3 shows schematically the (001) crystal plane of KCl with  $\text{Cl}_3^-$  molecules oriented along the  $[010]$  direction. In the lower right-hand corner of figure 3, a model of the  $\text{Cl}_3^-$  centre is shown in a lattice region undisturbed by other defects. The central portion of figure 3 displays the interaction of the centre with a dislocation for one of their possible mutual orientations. The Burgers vector of the dislocation is oriented along the  $[110]$  direction and the molecule experiences a tensile stress. In order to demonstrate more clearly the interaction of a dislocation with the  $\text{Cl}_3^-$  centre, we show in the inset in the lower left-hand corner of figure 3 an extremely simplified scheme for the same crystal plane with the defects. The scheme does not adhere to the true relationship between the radius of the Cl ion, the length of the  $\text{Cl}_3^-$  molecule, and

the lattice parameter; the cation sublattice is not shown. The letter  $a$  in the inset indicates a  $\text{Cl}_3^-$  centre far from a dislocation; the letter  $b$  denotes a centre involved in a direct interaction with the dislocation, just like in the main part of figure 3. It can be seen that the elastic interaction with the dislocation leads to extension of the molecule (in figure 3, the molecule is shown extended by 10%). The elongation of the molecular bonds requires an additional stress, which means that the  $\text{Cl}_3^-$  centres resist the dislocation motion. It can be understood from figure 3 that further motion of the dislocation in the same slip plane is impossible without rupture of the  $\text{Cl}_3^-$  molecule. If the intramolecular bonds were retained upon such a motion, the molecule would take on the configuration denoted by the letter  $c$  in the inset. This configuration is most probably unstable, because, in particular, it requires a bond elongation by  $\sim 50\%$  while estimates made below show that the bonds are ruptured at RT upon significantly weaker deformation.

We can determine the probability of dislocation-induced rupture of the  $\text{Cl}_3^-$  molecule in the following way. Atoms in the trihalide ion  $\text{Cl}_3^-$  are covalently bonded [14]. For such bonds, the dependence of the interatomic potential  $U$  on the interatomic distance  $r$  is well described by the relation  $U(r) = U_0 E(A)$ , where  $U_0$  is the energy of dissociation of the molecule;  $E$  is the Rydberg function:  $E(A) = -(I + A) \exp(-A)$ ;  $A = (r - r_0)/l$ ;  $r_0$  is the equilibrium interatomic distance;  $l = (U_0/k_0)^{1/2}$ ; and  $k_0$  is the force constant [15].  $U_0$  can be deduced from the TSL data. As mentioned above, the glow peak at 450 K is associated with the dissociation of  $\text{Cl}_3^-$  centres into H and  $\text{V}_F$  centres. The activation energy for this peak (1.25 eV [16]) is constituted by the dissociation energy of the  $\text{Cl}_3^-$  molecule  $U_0$  and the energy required for separation of the dissociation products. Since the migration energy of the H centre is only several hundredths of an electron volt, we can assume  $U_0 = 1.25$  eV.

The value of  $r_0$  can be estimated on the basis of the following considerations. The position of the absorption band for  $\text{Cl}_3^-$  centres is known [17] to coincide with that for the  $\text{Cl}_3^-$  molecules in a solution; hence, the crystal matrix deforms the  $\text{Cl}_3^-$  molecule only slightly. According to [14],  $r_0$  in the  $\text{X}_3^-$  molecule is approximately 10% longer than the bond length  $R$  in the corresponding molecule  $\text{X}_2^0$ . For  $\text{Cl}_2$ ,  $R = 2.01 \times 10^{-8}$  cm; hence,  $r_0 = 2.21 \times 10^{-8}$  cm. Finally,  $k_0 = 0.96$  N cm $^{-1}$  [14].

Now, given the  $U(r)$  function, we can determine the interatomic force  $f(r) = -dU(r)/dr$  and the maximum value of this force  $f_{\max}$ . We obtained  $f_{\max} = 1.6 \times 10^{-9}$  N; the bond elongation due to this force is 25%.

The force of elastic interaction between a dislocation and an obstacle cannot exceed  $Gb^2$  [18] (where  $G$  is the shear modulus and  $b$  is the Burgers vector). This force is directed along  $\langle 110 \rangle$  and its component in the direction of the molecule extension is only a fraction of the above value  $Gb^2$ . For KCl,  $G = 1.7 \times 10^6$  N cm $^{-2}$ ,  $b = 4.44 \times 10^{-8}$  cm; therefore,  $Gb^2 = 3.4 \times 10^{-9}$  N, so  $f_{\max} \sim Gb^2/2$ . Hence, there is little chance that a force  $f_{\max}$  will be applied by a dislocation to a  $\text{Cl}_3^-$  centre. At the same time, the tensile force  $P < f_{\max}$  can break the  $\text{Cl}_3^-$  molecule by the thermofluctuational mechanism [19].

The rate of thermally activated rupture of the stressed bonds is determined by the activation energy  $U_P < U_0$ . In the case under consideration,  $U_P$  is governed by the experimental conditions via the average time required for rupture:  $t_P = \tau_0 \exp(U_P/kT)$ , where  $\tau_0$  is the period of atomic vibration. It is obvious that  $t_P$  must not exceed the average time  $t_S$  spent by a dislocation in surmounting a single obstacle; otherwise, the dislocation would bypass the  $\text{Cl}_3^-$  centre, say, by the Orowan mechanism. In alkali halides,  $t_S \approx d/v$ , where  $d$  is the average spacing between obstacles and  $v$  is the average velocity of dislocation motion. The velocity  $v$  can be obtained from the plastic deformation equation  $\dot{\epsilon} = b\rho_m v$ , where  $\rho_m$  is the density of moving dislocations. For  $10^{18}$  cm $^{-3}$  concentration of  $\text{Cl}_3^-$  centres, we have  $d \sim 10^{-6}$  cm. Assuming that  $\rho_m \sim 10^8$  cm $^{-2}$ , we find  $t_S \sim 10^{-2}$  s. Finally, we obtain that the rate of bond



rupture is sufficiently high at 300 K if  $U_p \leq 0.6$  eV. Now, we can find the force of bond stretching  $P$ , which is necessary for the activation energy of bond rupture to be reduced from 1.25 to 0.6 eV. This force can be found from the expression [19]  $U_p = \int_{r_1}^{r_2} (f(r) - P) dr$ , where  $r_1$  and  $r_2$  are determined by the relationship  $f(r_1) = f(r_2)$ . As a result, we have  $P = 0.55 \times 10^{-9}$  N. The bond elongation is 10% in this case.

Thus, dissociation of  $\text{Cl}_3^-$  centres and consequently the DL are possible at RT if the tensile stress acting on a  $\text{Cl}_3^-$  molecule is about  $Gb^2/6$ . This value seems to be quite reasonable. If the  $\text{Cl}_3^-$  molecule is incorporated into a composite colour centre with lowered dissociation energy, e.g., a  $\text{V}_Z$  centre, the tensile stress may be even smaller.

The interpretation of DL as being a result of thermally activated destruction of  $\text{X}_3^-$  centres by dislocations makes it possible to explain all the DL features known for pure alkali halides, including the dependence of DL on temperature and strain rate. The latter dependence is described as  $I_{\text{DL}} \sim \dot{\epsilon}^{-\alpha}$  [4] ( $I_{\text{DL}}$  is the DL intensity;  $\alpha < 1$ ). Hence it follows that the number of photons emitted during the time corresponding to a unit deformation decreases with increasing  $\dot{\epsilon}$ . The reason may be that  $t_s$  decreases with increasing  $\dot{\epsilon}$ .

## 5. Conclusions

The above discussion led us to the following conclusions. Irradiation of alkali halides gives rise to hole-type colour centres formed by molecular ions  $\text{X}_2^-$  ( $\text{H}$ ,  $\text{V}_K$ , and  $\text{V}_F$  centres) and  $\text{X}_3^-$  ( $\text{V}_2$  and  $\text{V}_Z$  centres). The atoms incorporated into such centres are noticeably displaced from their normal lattice positions. The distance between two halide atoms decreases by 40% when a  $\text{V}_K$  centre is formed [20], and even greater decrease is expected for  $\text{V}_2$  centres. The changes in the interatomic distances, along with changes in the charge state of the atoms, lead to lattice distortion in the vicinity of these colour centres, which undoubtedly hinders dislocation slip. However, when considering the mechanism of irradiation-induced strengthening of alkali halides, we should take into account not only the lattice distortions, but also the formation of chemical bonds untypical of the regular lattice. A dislocation cannot cut through a hole centre without rupture of intramolecular bonds (in the case of  $\text{X}_3^-$  centres) or without reorientation of the centre (in the case of  $\text{X}_2^-$  centres). At RT,  $\text{X}_3^-$  centres are predominant in alkali halides. In KCl crystals (as, seemingly, also in other chlorides), the intramolecular bonds in  $\text{Cl}_3^-$  centres are so strong that the stress required for their rupture is comparable with the maximum possible local stress. Most probably, it is the formation of covalent bonds that is responsible for the strengthening of alkali halides upon RT irradiation to moderate doses (until large defects are formed).

Dissociation of  $\text{Cl}_3^-$  centres gives rise to pairs of mobile H and  $\text{V}_F$  centres. Since these centres escape from the place where a dislocation was pinned by the obstacle, the regular lattice is restored there. The recombination of the mobile centres with F-type centres results in light emission, which is detected as DL. It should be mentioned that the origin of DL cannot be reduced to just stress-assisted dissociation of hole centres. The dislocations can not only destroy these centres, but also displace them through small distances. The above-mentioned reorientation of  $\text{X}_2^-$  centres can serve as an example of such a displacement. As another example, an F centre can be shifted owing to the deformation shear by a single interatomic distance. For some close pairs of electron and hole centres, such a displacement may be sufficient to provide recombination; the low-intensity DL observed after annealing of  $\text{X}_3^-$  centres might originate from this process.

Thus, the main conclusions of this study can be formulated as follows. Point defects that exert a strengthening effect on KCl crystals upon RT irradiation are  $\text{Cl}_3^-$  centres. The interaction of these centres with a moving dislocation results in their dissociation and consequently in the DL.



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