

## Correlation between deformation bleaching and mechanoluminescence in coloured alkali halide crystals

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**Abstract.** The present paper reports the correlation between deformation bleaching of coloration and mechanoluminescence (ML) in coloured alkali halide crystals. When the  $F$ -centre electrons captured by moving dislocations are picked up by holes, deep traps and other compatible traps, then deformation bleaching occurs. At the same time, radiative recombination of dislocation captured electrons with the holes gives rise to the mechanoluminescence. Expressions are derived for the strain dependence of the density of colour centres in deformed crystals and also for the number of colour centres bleached. So far as strain, temperature, density of colour centres,  $E_a$  and volume dependence are concerned, there exists a correlation between the deformation bleaching and ML in coloured alkali halide crystals. From the strain dependence of the density of colour centres in deformed crystals, the value of coefficient of deformation bleaching  $D$  is determined and it is found to be 1.93 and 2.00 for KCl and KBr crystals, respectively. The value of  $(D + \chi)$  is determined from the strain dependence of the ML intensity and it is found to be 2.6 and 3.7 for KCl and KBr crystals, respectively. This gives the value of coefficient of deformation generated compatible traps  $\chi$  to be 0.67 and 1.7 for KCl and KBr crystals, respectively.

**Keywords.** Deformation bleaching; colour centres; alkali halides.

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### 1. Introduction

The phenomenon of mechanoluminescence (ML), i.e., the light emission produced during deformation of solids, was reported in coloured alkali halide crystals for the first time in 1930 by Urbach [1]. Trinks [2] found the increase in ML intensity of NaCl and KCl crystals with irradiation doses, thickness of the crystals and with the pressure. Wick [3] also reported the ML emission during deformation of coloured alkali halide crystals. The linear dependence of light emission on the strain rate in  $X$ -irradiated KBr, NaCl and LiF crystals was reported by Metz *et al* [4] and Alzetta *et al* [5]. The decrease in ML intensity with increasing rate of compression was reported by Pirog and Sujak [6]. Leider [7] and Senchukov and Shmurak [8] have shown independently that the ML occurs in most of the cases due to the recombination of free electrons with the luminescence centres. Several workers have reported the dislocation movement to be responsible for the ML excitation

in coloured alkali halide crystals [9]. Butler [10] has shown that the ML spectra of  $\gamma$ -irradiated alkali halide crystals are similar to the luminescence excited by high energy radiation. Ueta *et al* [11] have shown that the decay curve of the electric current produced during plastic deformations of non-irradiated KCl crystals and the decay curve of the ML produced during deformation of the irradiated crystals are of the same form. Chandra and Elyas [12] have reported that the ML is produced in coloured alkali halide crystals during the application of pressure as well as during the release of applied pressure. Guerrero and Alvarez Rivas [13] have studied the dependence of ML and thermoluminescence on the strain of irradiated KCl crystals. Hardy *et al* [14] have reported that the ML excited by 1060 nm Nd glass laser beam is similar in spectra to the ML excited by plastic deformations of  $X$  or  $\gamma$ -irradiated alkali halide crystals. Mayer and Winnacker [15] have reported the ML and thermoluminescence in  $\gamma$ -irradiated KCl crystals. Miyake and Futama [16] have studied the effect of annealing in chlorine gas on the ML of X-rayed KCl crystals. Ossipyan and Shmurak [17], Molotskii [18] and Molotskii and Shmurak [19] have studied the mechanism of ML excitation in coloured alkali halide crystals. Hagihara *et al* [20] and Hayashiuchi *et al* [21] have also investigated the process of ML excitation in  $\gamma$ -irradiated KCl crystals. Atari [22], Copty-Wergles *et al* [23], Poletaev and Shmurak [24], Eid *et al* [25] and Al-Hashmi *et al* [26] have reported the dependence of the ML of coloured alkali halide crystals on different parameters. Zakrevskii and Shuldiner [27] have studied the electron emission and luminescence associated with the plastic deformation of ionic crystals. Chandra [28,29] has reported the dependence of ML of coloured alkali halide crystals on different parameters. Several workers have reported that post-irradiation deformation causes deformation bleaching in coloured alkali halide crystals [17,30–38].

Since the post-irradiation deformation causes bleaching of coloration and the ML emission, a correlation between the deformation bleaching and mechanoluminescence of coloured alkali halide crystals is expected. The present paper reports the correlation between the deformation bleaching and ML in coloured alkali halide crystals.

## 2. Theory

### 2.1 Expression for the dependence of deformation bleaching on different parameters

When a coloured alkali halide crystal is plastically deformed, movement of dislocations takes place. The moving dislocations may capture electrons from the colour centres and may subsequently transport the captured electrons to hole centres, deep traps and other compatible traps in the crystal. As a matter of fact, deformation bleaching of the coloration in alkali halide crystals may take place. Suppose a crystal contains  $N_d$  dislocations of unit length per unit volume. When  $N_d$  dislocations move through a distance  $dx$ , then the area swept out by the dislocations will be  $N_d dx$ . The deformation bleaching in coloured alkali halide crystals may take place due to the transfer of electrons from  $F$ -centres to the dislocation band and their subsequent recombination with other centres.

It has been shown in our previous paper [30] that the density  $n_F$  of the  $F$ -centres in coloured alkali halide crystals decreases with post-irradiation deformation of the crystals, and the dependence of  $n_F$  on the strain  $\varepsilon$  may be expressed as

$$n_F = n_{FO} \exp(-D\varepsilon), \quad (1)$$

where  $D$  is the coefficient of deformation bleaching given by

$$D = \frac{p_F r_F}{b}$$

in which  $r_F$  is the distance up to which a dislocation can interact with colour centre,  $p_F$  is the dislocation capture-probability of  $F$ -centre electrons and  $b$  is Burgers vector.  $n_{FO}$  is the density of  $F$ -centres in the undeformed crystal, and  $\varepsilon$  is strain or deformation.

For a crystal of volume  $V$ , eq. (1) may be expressed as

$$n'_F = n_F V = n_{FO} V \exp(-D\varepsilon). \quad (2)$$

Thus, the number of colour centres bleached in a crystal of volume  $V$  at deformation  $\varepsilon$  may be expressed as

$$\Delta n_F = n_{FO} V [1 - \exp(-D\varepsilon)]. \quad (3)$$

## 2.2 Expressions for the dependence of ML on different parameters

When a coloured alkali halide crystal is deformed, the moving dislocations capture electrons from the nearby  $F$ -centres. It is to be noted that the dislocation band lies just above the ground state of  $F$ -centre level [39,40]. It has been shown in our previous investigation that the rate of generation of electrons in the dislocation band may be expressed by the relation [30]

$$g = \frac{\dot{\varepsilon}}{b} p_F r_F n_F, \quad (4)$$

where  $\dot{\varepsilon}$  is the strain rate of the crystal.

From eqs (1) and (4), we get

$$g = \frac{p_F n_{FO} r_F \dot{\varepsilon}}{b} \exp(-D\varepsilon)$$

or

$$g = g_0 \exp(-D\varepsilon), \quad (5)$$

where

$$g_0 = \frac{p_F n_{FO} r_F \dot{\varepsilon}}{b}. \quad (6)$$

When the moving dislocations containing electrons encounter defect-centres like hole centres, deep traps and other compatible traps, the electrons are captured by these centres. As such, the rate equation may be written as

$$\frac{dn_d}{dt} = g - \sigma_1 N_1 v_d n_d - \sigma_2 N_2 v_d n_d - \sigma_3 N_3 v_d n_d, \quad (7)$$

where  $n_d$  is the number of electrons in the dislocation band at any time  $t$ ,  $\sigma_1$ ,  $\sigma_2$  and  $\sigma_3$  are the cross-sections and  $N_1$ ,  $N_2$  and  $N_3$  are the densities of hole centres, deep traps and other

compatible traps, respectively and  $v_d$  is velocity of dislocations. The velocity of electrons has been taken as the velocity of dislocations because the dislocation captured electrons move with the dislocations. Here, the compatible traps means the traps whose electron capture-probability is much greater than that of dislocations. It should be noted that the vacant negative ion vacancies have nearly the same probability of electron-capturing and electron-detrapping, hence, their presence may not affect significantly the recombination process.

From eqs (5) and (7), we get

$$\frac{dn_d}{dt} = g_0 \exp(-D\varepsilon) - \gamma n_d \quad (8)$$

or

$$\frac{dn_d}{dt} = g_0 \exp(-D\dot{\varepsilon}t) - \gamma n_d,$$

where

$$\gamma = \frac{1}{\tau_d} = (\sigma_1 N_1 + \sigma_2 N_2 + \sigma_3 N_3) v_d. \quad (9)$$

where  $v_d$  is the lifetime of electrons in the dislocation band.

By integrating eq. (8) and taking  $n_d = 0$ , at  $t = 0$ , we get

$$n_d = \frac{g_0}{(\gamma - D\dot{\varepsilon})} [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]. \quad (10)$$

From eq. (7), the rate of the recombination of dislocation electrons with holes may be given by

$$R_h = \sigma_1 N_1 v_d n_d$$

or

$$R_h = \frac{\sigma_1 N_1 v_d g_0}{(\gamma - D\dot{\varepsilon})} [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]. \quad (11)$$

Substituting the value of  $v_d$  from eq. (9), we get

$$R_h = \frac{\sigma_1 N_1 g_0 \gamma}{(\sigma_1 N_1 + \sigma_2 N_2 + \sigma_3 N_3)(\gamma - D\dot{\varepsilon})} [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]. \quad (12)$$

As the number of deep traps is less as compared to other centres, we get

$$R_h = \frac{\sigma_1 N_1 g_0 \gamma}{(\sigma_1 N_1 + \sigma_3 N_3)(\gamma - D\dot{\varepsilon})} [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]$$

or

$$R_h = \frac{g_0 \gamma}{\left(1 + \frac{\sigma_3 N_3}{\sigma_1 N_1}\right) (\gamma - D\dot{\varepsilon})} [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]. \quad (13)$$

It is known that the electron-traps are created by the plastic deformation of alkali halide crystals whose density increases more or less linearly with the deformation of crystals [34].

Thus the dependence of the number  $N_\varepsilon$  of newly created electron traps due to the strain may be expressed as

$$N_\varepsilon = M\varepsilon,$$

where  $M$  is the multiplication factor.

Out of the deformation generated  $N_\varepsilon$  electron traps, a fraction  $A$  of them may have electron capture-probability greater than that of dislocations and thus the number of deformation-generated compatible electron traps  $N_3$  may be given by

$$N_3 = AM\varepsilon. \quad (14)$$

Thus, eq. (13) may be written as

$$R_h = \frac{g_0\gamma}{(1 + \chi\varepsilon)(\gamma - D\dot{\varepsilon})} [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)], \quad (15)$$

where

$$\chi = \frac{\sigma_3 AM}{\sigma_1 N_1}$$

is the coefficient of deformation-generated compatible traps.

When  $\chi\varepsilon$  is less than 1, eq. (15) may be written as

$$R_h = \frac{g_0\gamma}{(\gamma - D\dot{\varepsilon})} \exp(-\chi\varepsilon) [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]. \quad (16)$$

For low deformation, the probability  $\eta$  of the radiative recombination of electrons with hole centres may be assumed to be a constant. Thus, the ML intensity may be expressed as

$$I = \eta R_h, \\ I = \frac{\eta\gamma g_0}{(\gamma - D\dot{\varepsilon})} \exp(-\chi\varepsilon) [\exp(-D\dot{\varepsilon}t) - \exp(-\gamma t)]. \quad (17)$$

Substituting the value of  $g_0$  from eq. (6) in eq. (17), we get

$$I = \frac{\eta\gamma P_F n_{FO} r_F \dot{\varepsilon}}{(\gamma - D\dot{\varepsilon})b} \exp(-\chi\varepsilon) [\exp(-D\varepsilon) - \exp(-\gamma\varepsilon/\dot{\varepsilon})]$$

or

$$I = \frac{\eta\gamma P_F n_{FO} r_F \dot{\varepsilon}}{(\gamma - D\dot{\varepsilon})b} \{ \exp[-(D + \chi)\varepsilon] - \exp[-(\gamma/\dot{\varepsilon} + \chi)\varepsilon] \}. \quad (18)$$

*Rise of ML intensity:* For low value of  $\varepsilon$ , eq. (18) may be written as

$$I = \frac{\eta\gamma P_F n_{FO} r_F \dot{\varepsilon}}{(\gamma - D\dot{\varepsilon})b} \left[ \frac{\gamma}{\dot{\varepsilon}} + \chi - D - \chi \right] \varepsilon$$

or

$$I = \frac{\eta\gamma P_F n_{FO} r_F \dot{\varepsilon}}{b}. \quad (19)$$

Equation (19) indicates that for low value of  $\varepsilon$ , the ML intensity should increase linearly with the strain  $\varepsilon$ .

*Maximum value of ML intensity:* Equation (18) shows that  $I = 0$  at  $\varepsilon = 0$  and  $I = 0$  at  $\varepsilon = \infty$ . Thus, the ML intensity should be maximum for a particular value of the strain. By equating  $dI/d\varepsilon = 0$ , we can get the value of strain  $\varepsilon_m$  at which ML intensity will be maximum. From eq. (18), we get

$$(D + \chi) \exp[-(D + \chi)\varepsilon] = (\chi + \gamma/\dot{\varepsilon}) \exp \left[ - \left( \chi + \frac{\gamma}{\dot{\varepsilon}} \right) \varepsilon \right]$$

or

$$\exp[-(D + \chi)\varepsilon] = \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)} \exp \left[ - \left( \chi + \frac{\gamma}{\dot{\varepsilon}} \right) \varepsilon \right]. \quad (20)$$

Writing  $\varepsilon = \varepsilon_m$  from eq. (20), we get

$$\exp[\chi + \gamma/\dot{\varepsilon} - D - \chi]\varepsilon_m = \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)}$$

or

$$\varepsilon_m = \frac{1}{(\gamma/\dot{\varepsilon} - D)} \ln \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)}. \quad (21)$$

From eqs (18) and (20) we get the maximum value of  $I = I_m$  as

$$I_m = \frac{\eta\gamma p_F n_{FO} r_F \dot{\varepsilon}}{(\gamma - D\dot{\varepsilon})b} \left\{ \exp[-(\chi + \gamma/\dot{\varepsilon})\varepsilon_m] \left[ \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)} - 1 \right] \right\}. \quad (22)$$

Substituting the value of  $\varepsilon_m$  from eq. (21) in eq. (22), we get

$$I_m = \frac{\eta\gamma p_F n_{FO} r_F \dot{\varepsilon}}{(\gamma - D\dot{\varepsilon})b} \times \left\{ \exp \left[ - \frac{(\chi + \gamma/\dot{\varepsilon})}{(\gamma/\dot{\varepsilon} - D)} \ln \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)} \right] \left[ \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)} - 1 \right] \right\}. \quad (23)$$

For  $\gamma \gg D\dot{\varepsilon}$  and  $\gamma \gg \chi\dot{\varepsilon}$ , eq. (23) may be expressed as

$$I_m = \frac{\eta p_F n_{FO} r_F \dot{\varepsilon}}{b} \left\{ \frac{(D + \chi)}{(\chi + \gamma/\dot{\varepsilon})} \frac{(\chi + \gamma/\dot{\varepsilon} - D - \chi)}{(D + \chi)} \right\}$$

or

$$I_m \approx \frac{\eta p_F n_{FO} r_F \dot{\varepsilon}}{b}. \quad (24)$$

As  $\gamma \gg \chi\dot{\varepsilon}$ , for large value of  $\varepsilon$ , eq. (18) may be expressed as

$$I = \frac{\eta p_F n_{FO} r_F \dot{\varepsilon}}{b} \exp[-(D + \chi)\varepsilon]. \quad (25)$$

Equation (25) indicates that for large deformation,  $I$  should decrease exponentially with  $\varepsilon$ .

From eq. (18), the total ML intensity  $I_T$ , i.e., the total number of photons emitted up to the strain  $\varepsilon$  of the crystal may be expressed as

$$I_T = \int_0^\varepsilon I d\varepsilon$$

or

$$I_T = \frac{\eta p_F n_{FOR} r_F \dot{\varepsilon}}{(\gamma - D\dot{\varepsilon})b} \int_0^\varepsilon \left\{ \exp[-(D + \chi)\varepsilon] - \exp\left[-\left(\frac{\gamma}{\dot{\varepsilon}} + \chi\right)\varepsilon\right] \right\} d\varepsilon.$$

As ( $\gamma \gg D\dot{\varepsilon}$ ), we have

$$I_T = \frac{\eta p_F n_{FOR} r_F \dot{\varepsilon}}{b} \int_0^\varepsilon \left\{ \exp[-(D + \chi)\varepsilon] - \exp\left[-\left(\chi + \frac{\gamma}{\dot{\varepsilon}}\right)\varepsilon\right] \right\} d\varepsilon$$

or

$$I_T = \frac{\eta p_F n_{FOR} r_F \dot{\varepsilon}}{b} \left\{ \frac{\exp[-(\chi + D)\varepsilon]}{-(D + \chi)} \right\}_0^\varepsilon - \left\{ \frac{\exp\left[-\left(\chi + \frac{\gamma}{\dot{\varepsilon}}\right)\varepsilon\right]}{-\left(\chi + \frac{\gamma}{\dot{\varepsilon}}\right)} \right\}_0^\varepsilon. \quad (26)$$

As  $((\chi + \gamma)/\dot{\varepsilon}) \gg (D + \chi)$ , the second term on the right hand side of the above equation may be neglected and we get

$$I_T = \frac{\eta p_F n_{FOR} r_F \dot{\varepsilon}}{b(D + \chi)} \{1 - \exp[-(D + \chi)\varepsilon]\}$$

or

$$I_T = I_T^0 \{1 - \exp[-(D + \chi)\varepsilon]\}, \quad (27)$$

where

$$I_T^0 = \frac{\eta p_F n_{FOR} r_F \dot{\varepsilon}}{b(D + \chi)}.$$

Equation (27) indicates that the total number of photons emitted should initially increase linearly with the deformation of crystals and then it should attain a saturation value for large deformation.

The probability  $p_F$  of the transfer of electrons from an  $F$ -centre to the interacting dislocation is related to the transfer of the electrons from the interacting  $F$ -centres to the dislocation band and its temperature dependence may be given by

$$p_F = p_F^0 \exp[-E_a/kT], \quad (28)$$

where  $E_a$  is the energy gap between the bottom of dislocation band and average ground state energy of the interacting  $F$ -centres and  $p_F^0$  is a constant.

From eqs (21), (27) and (28), we get

$$I_m = \frac{\eta n_{FOR} r_F \dot{\varepsilon} p_F^0}{b} \exp[-E_a/kT] \quad (29)$$

and

$$I_T = \frac{\eta n_{FO} r_F \dot{\epsilon} p_F^0}{b(D + \chi)} \exp[-E_a/kT] \{1 - \exp[-(D + \chi)\epsilon]\}. \quad (30)$$

Equations (29) and (30) show that for given values of  $n_{FO}$  and  $\dot{\epsilon}$ , both  $I_m$  and  $I_T$  should increase with temperature of the crystal, following Arrhenius plot with an activation energy  $E_a$ . However, at higher temperature  $n_{FO}$  will decrease due to the thermal bleaching and thereby  $I_m$  and  $I_T$  should be optimum for a particular temperature of the crystals.

### 2.3 Correlation between the deformation bleaching and ML in coloured alkali halide crystals

When the  $F$ -centre electrons captured by moving dislocations are picked up by holes, deep traps and other compatible traps, then deformation bleaching occurs. At the same time, radiative recombination of dislocation captured electrons with the holes gives rise to the mechanoluminescence. Thus, there should be a correlation between deformation bleaching and ML.

- (i) It has been found (eq. (3)) that the deformation bleaching may be given by

$$\Delta n_F = n_{FO} V [1 - \exp(-D\epsilon)].$$

However, the total number of photons emitted may be given by (eq. (27))

$$I_T = I_T^0 [1 - \exp-(D + \chi)\epsilon].$$

Thus, the strain dependence of deformation bleaching is slower as compared to the strain dependence of total ML intensity. From the strain dependence of deformation bleaching, the coefficient of deformation bleaching  $D$  may be calculated and using this value of  $D$ , the coefficient of deformation generated compatible traps  $\chi$  may be determined from the strain dependence of  $I_T$ .

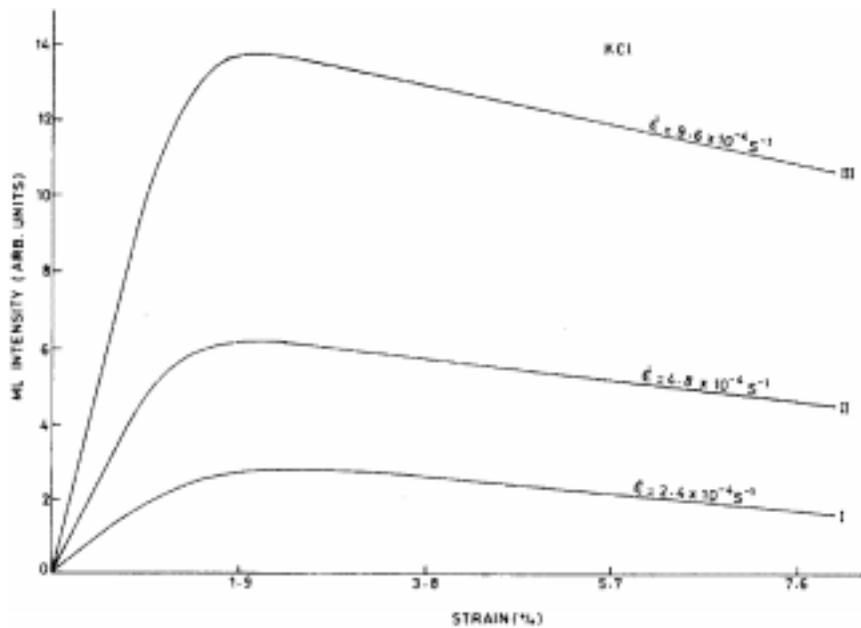
- (ii) Whereas the ML intensity depends linearly on the strain rate ( $\dot{\epsilon}$ ), (eq. (19)), the deformation bleaching weakly depends on the  $\dot{\epsilon}$  depending on the strain rate dependence of  $D$  (eq. (1)).
- (iii) Both the deformation bleaching and mechanoluminescence should initially increase with the increasing temperature of the crystal because of the increase in the dislocation capture probability of  $F$ -centre electrons and both of them should decrease at high temperature because of the thermal bleaching of the coloration in alkali halide crystals. Thus, both the deformation bleaching and mechanoluminescence intensity should be optimum for a particular temperature of the crystals.
- (iv) Both the deformation bleaching and ML should depend linearly on the density of colour centres in the undeformed crystals.
- (v) Since both the deformation bleaching and mechanoluminescence depends on the dislocation capture probability of  $F$ -centre electrons, which decreases with the increasing value of  $E_a$ , i.e., the energy gap between the dislocation band and ground state of  $F$ -centre electrons, they should consequently decrease with increasing value of  $E_a$ .

- (vi) Both the deformation bleaching and mechanoluminescence intensity should increase with the volume  $V$  of the crystals.

### 3. Experimental support to the proposed theory

For getting the experimental support to the theory proposed for the correlation between deformation bleaching and mechanoluminescence, pure single crystals of KCl, KBr and NaCl were grown using melt technique. Specimens of size  $5 \times 5 \times 5 \text{ mm}^3$  were cleaved. Before irradiation, the crystals were annealed at  $450^\circ\text{C}$  for two hours. The  $\gamma$ -irradiation was carried out at room temperature using  $^{60}\text{Co}$  source.

The optical density of coloured crystal is measured after different values of deformation by using a Shimadzu double-beam UV-240 spectrophotometer. The density of  $F$ -centres is determined using Smakula's formula. While high energy  $\gamma$ -irradiation produces  $F$ -centres in regions of high local density, for the comparison of the experimental results with the phenomenological model, a statistical distribution was assumed. It is to be noted that  $p_F$  and  $r_F$  are independent of the density of  $F$ -centres, hence, a non-uniform distribution of  $F$ -centres may not affect their values. For the ML measurement, the crystals were deformed along (100) direction by using tensile tester (Model 1.3 KMI, Ahmedabad) where the strain rate could be taken as  $2.4 \times 10^{-4} \text{ s}^{-1}$ ,  $4.8 \times 10^{-4} \text{ s}^{-1}$ ,  $9.6 \times 10^{-4} \text{ s}^{-1}$ . In this technique, the ML intensity was measured by using an RCA 931A photomultiplier tube whose output was connected to a  $X$ - $Y$  recorder. The strain was estimated from the known speed of cross-head in the device which compresses the crystal. The measurement was carried out in a dark room.

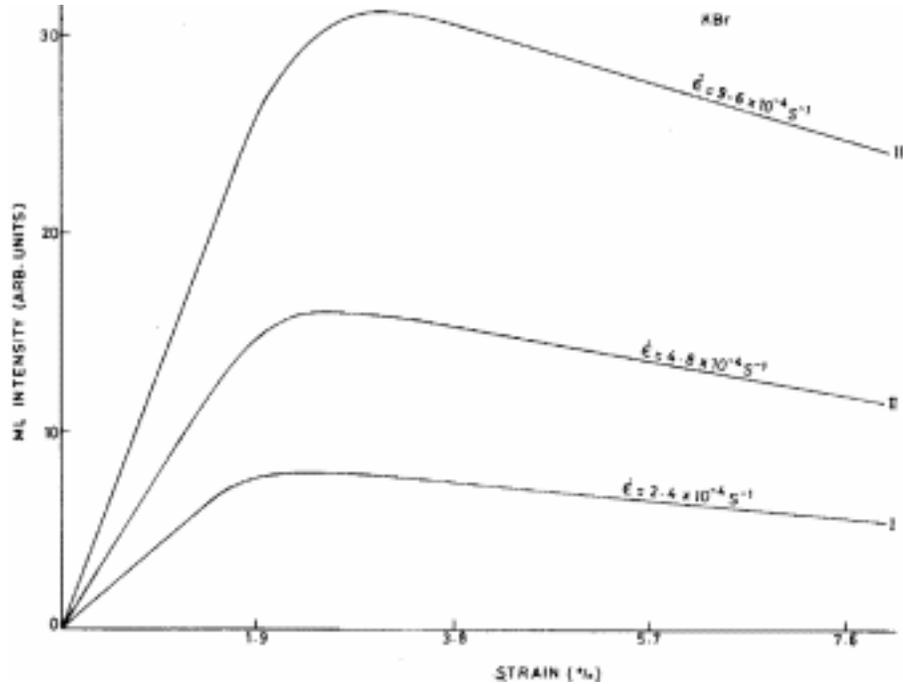


**Figure 1.** Dependence of ML intensity on the strain for  $\gamma$ -irradiated KCl crystals (dimension =  $5 \times 5 \times 5 \text{ mm}^3$ ,  $n_F \approx 10^{17} \text{ cm}^{-3}$ ).

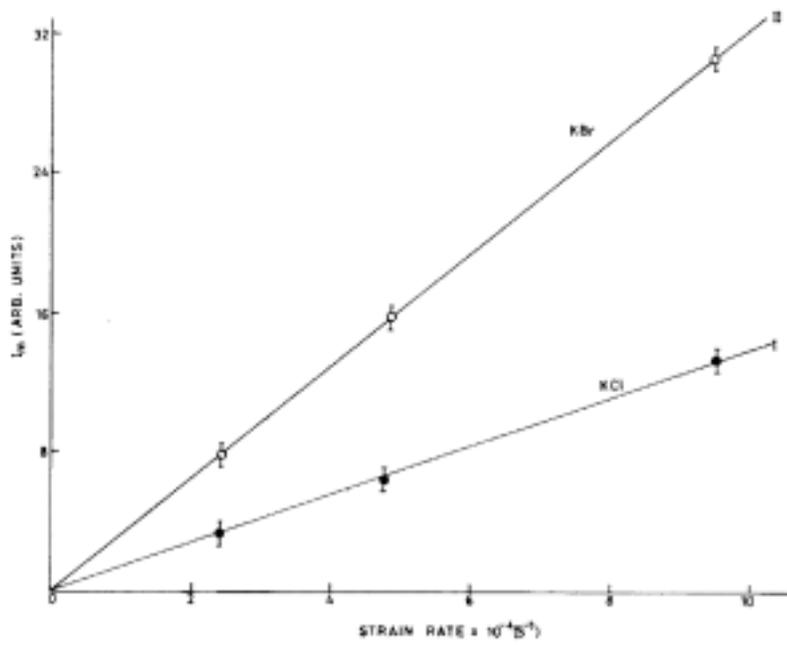
It has been reported in our earlier investigation [30] that the density of  $F$ -centres decreases with the deformation of crystals, and the plot of  $\ln(n_F)$  versus strain is a straight line with a negative slope. From the plot between  $\ln(n_F)$  and  $\varepsilon$ , slope has been determined. It has been found to be 1.9, 1.69 and 1.7 for KBr, KCl and NaCl crystals, respectively.

Figures 1 and 2 show the dependence of ML intensity on the strain for  $\gamma$ -irradiated KCl and KBr crystals, respectively. It is seen that initially the ML intensity increases with the deformation, attains an optimum value and then it decreases with further deformation of the crystal. It is seen that the peak of ML intensity versus strain curve shifts towards higher strain values with increasing strain rate of the crystals. The results shown in figures 1 and 2 follow eq. (21). It is seen from figure 3 that the peak of the ML intensity  $I_m$  of  $\gamma$ -irradiated KCl and KBr crystals increases linearly with the strain rate. Equation (24) supports such dependence of  $I_m$  on  $\dot{\varepsilon}$ .

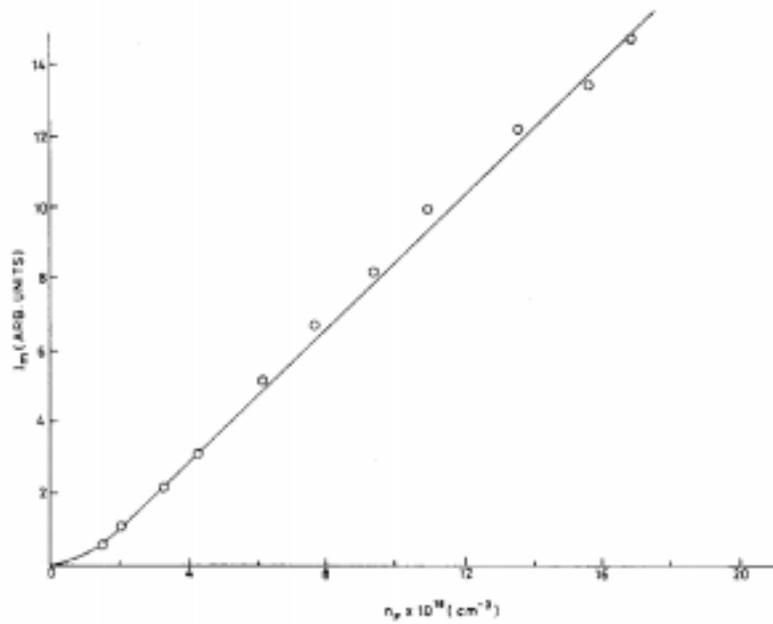
The dependence of the peak of ML intensity versus strain curve on the density of  $F$ -centres is shown in figure 4. It is seen that  $I_m$  increases linearly with the density of  $F$ -centres. This fact is in accord with eq. (24). Figures 5 and 6 show that for higher value of strain, the plot of  $\log I$  versus  $\varepsilon$  are straight lines with negative slopes. This result supports eq. (25). The value of slope, i.e.,  $(D + \chi)$  is found to be 2.6 and 3.7 for KCl and KBr crystals, respectively.



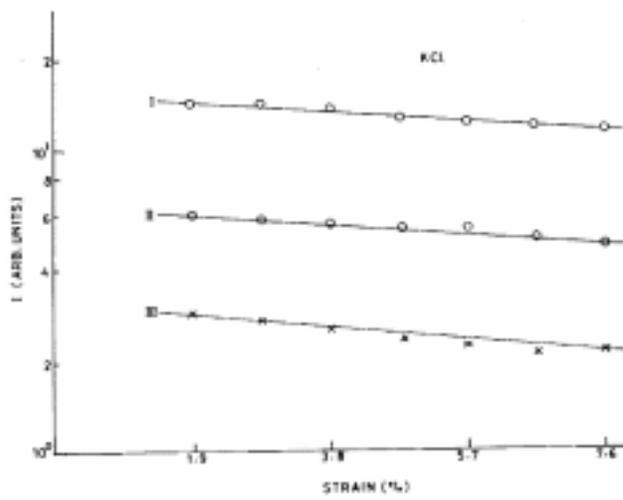
**Figure 2.** Dependence of ML intensity on the strain ( $\varepsilon$ ) for  $\gamma$ -irradiated KBr crystals (dimension =  $5 \times 5 \times 5 \text{ mm}^3$ ,  $n_F \approx 10^{17} \text{ cm}^{-3}$ ).



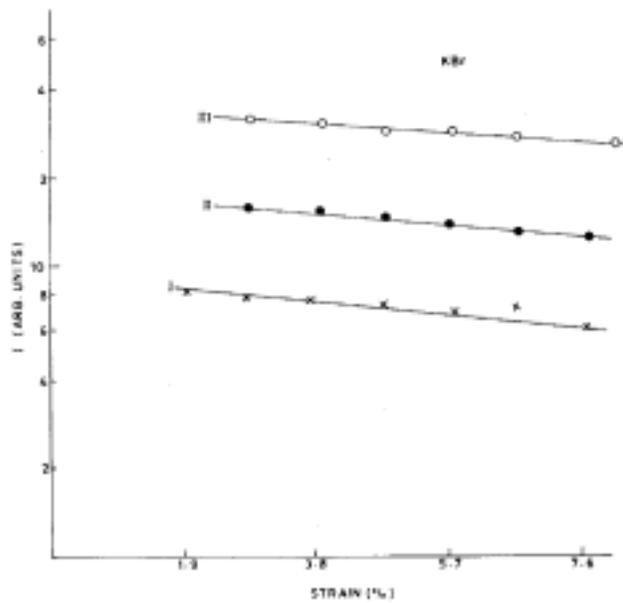
**Figure 3.** Dependence of ML intensity on the strain rate ( $\dot{\epsilon}$ ) for  $\gamma$ -irradiated KCl and KBr crystals (dimension =  $5 \times 5 \times 5 \text{ mm}^3$ ,  $n_F \approx 10^{17} \text{ cm}^{-3}$ ).



**Figure 4.** Dependence of ML intensity on the density of  $F$ -centres in KCl crystal (dimension =  $5 \times 5 \times 5 \text{ mm}^3$ ).

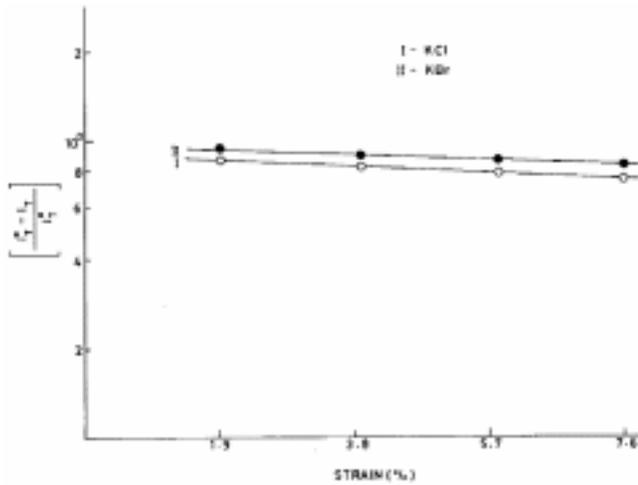


**Figure 5.** Plot of  $\log I$  versus strain for  $\gamma$ -irradiated KCl crystals (dimension =  $5 \times 5 \times 5$  mm<sup>3</sup>,  $n_F \approx 10^{17}$  cm<sup>-3</sup>). I, II and III correspond to different strain rates described previously.

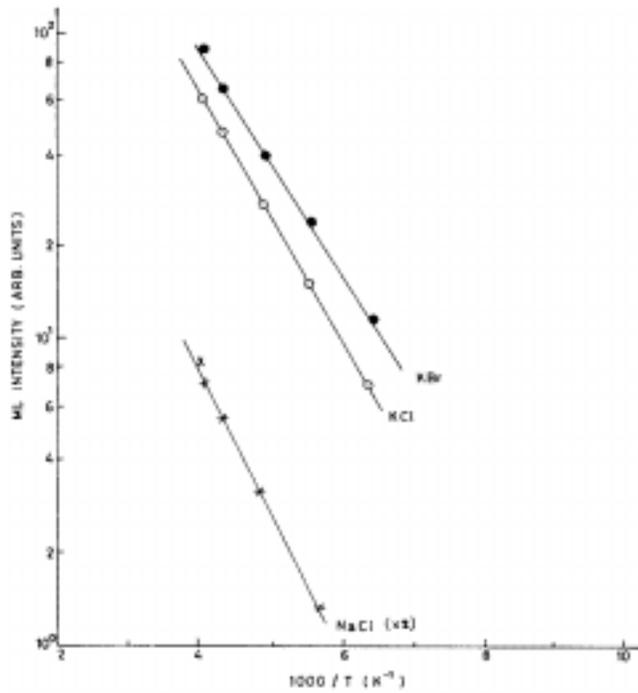


**Figure 6.** Plot of  $\log I$  versus strain for  $\gamma$ -irradiated KBr crystals (dimension =  $5 \times 5 \times 5$  mm<sup>3</sup>,  $n_F \approx 10^{17}$  cm<sup>-3</sup>). I, II and III correspond to different strain rates described previously.

Figure 7 shows that the plot of  $\log [(I_T^0 - I_T)/I_T^0]$  versus strain  $\epsilon$  is a straight line with a negative slope. From the slope of  $\log [(I_T^0 - I_T)/I_T^0]$  versus  $\epsilon$  curve, the value of  $(D + \chi)$



**Figure 7.** Plot of  $\log [(I_T^0 - I_T) / I_T^0]$  versus strain for  $\gamma$ -irradiated KCl and KBr crystals (dimension =  $5 \times 5 \times 5 \text{ mm}^3$ ,  $n_F \approx 10^{17} \text{ cm}^{-3}$ ).



**Figure 8.** Plot of  $\log I$  versus  $1000/T$  for  $\gamma$ -irradiated KCl, KBr and NaCl crystals ( $n_F \approx 10^{17} \text{ cm}^{-3}$ ,  $\dot{\epsilon} = 10^{-4} \text{ s}^{-1}$ ).

is found to be 2.6 and 2.9 for KCl and KBr crystals, respectively. In this case, the value of  $I_T^0$  is determined from  $I_T^0 = I_m / (D + \chi)$ .

Figure 8 shows that the plot of  $\log I_m$  versus  $1000/T$  is a straight line with a negative slope. Such prediction is made from eq. (29). The value of  $E_a$  is found to be 0.07, 0.075 and 0.080 eV for KCl, KBr and NaCl crystals, respectively. Figure 9 shows the ML spectra of  $\gamma$ -irradiated KCl, KBr and NaCl crystals, respectively, recorded using 1/2 m Bausch and Lomb grating monochromator [41]. It is seen that the peaks of the ML spectra lie at 455, 463, 450 nm for KCl, KBr and NaCl crystals, respectively.

It has been proposed that the ML emission is due to the recombination of  $F$ -centre electrons with the  $V_2$ -hole centres. Thus, the energy corresponding to the peak of the ML spectra should correspond to the difference between the bottom of the conduction band and the energy level of  $V_2$  centres ( $E_{v_2}$ ) (figure 10). The wavelength  $\lambda_m$  corresponding to the peak of ML spectra is calculated from the relation  $\lambda_m = [ch/(E_c - E_{v_2})]$ , where  $c$  is the velocity of light and  $h$  is the Planck constant. A good agreement is found between the calculated value of  $\lambda_m$  and the experimentally observed value of the  $\lambda_m$ . It is to be noted that the ML spectrum is illustrated in figure 9. It has features which are different both qualitatively and quantitatively from those reported by Butler [10]. This difference may be due to the differences in the quality of crystals and also in the quality of the instrumentations used, i.e., the monochromator and photomultiplier used. The spectra shown in figure 9 approximates with the ML spectra reported by Atari [22].

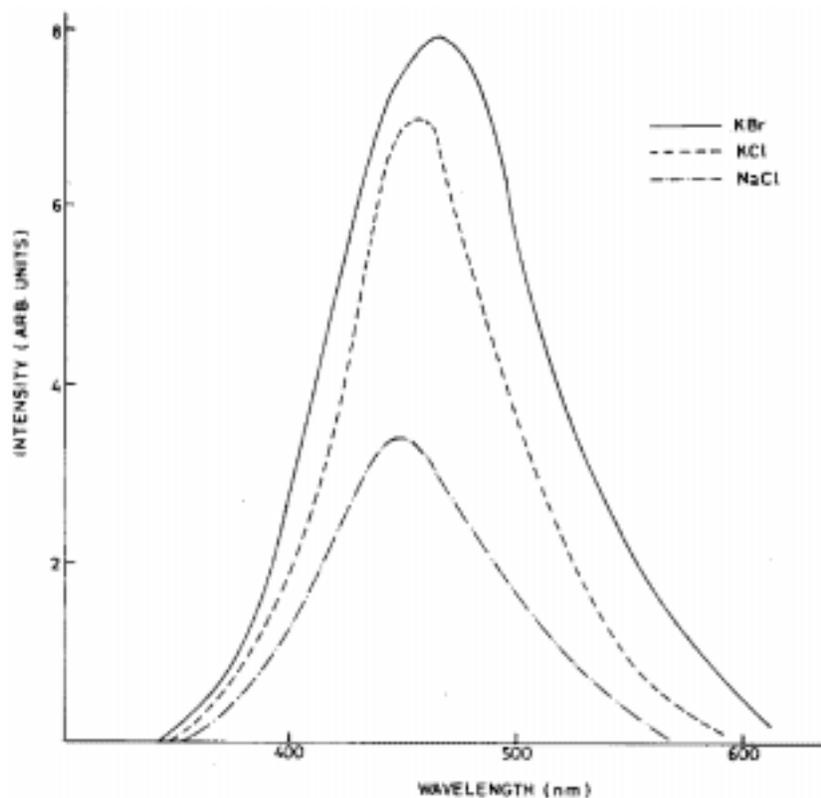
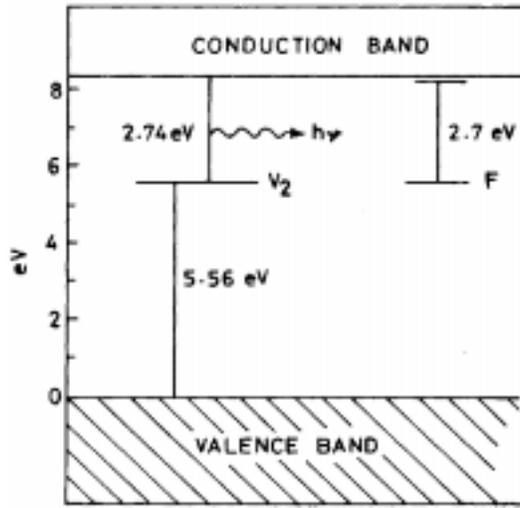


Figure 9. ML spectra of  $\gamma$ -irradiated NaCl, KCl and KBr crystals.



**Figure 10.** Energy level diagram showing ML processes involving  $V_2$  and  $F$ -centres in NaCl.

#### 4. Conclusions

- (i) When the  $F$ -centre electrons captured by moving dislocations are picked up by holes, deep traps and other compatible traps, then deformation bleaching occurs. At the same time, radiative recombination of dislocation captured electrons with the holes gives rise to the mechanoluminescence. Thus, there should be correlation between deformation bleaching and mechanoluminescence.
- (ii) Expressions are derived for the strain dependence of the density of colour centres in deformed crystals, and also for the number of colour centres bleached, which are respectively as given below:

$$n_F = n_{FO}V \exp(-D\varepsilon)$$

and

$$\Delta n_F = n_{FO}V [1 - \exp(-D\varepsilon)].$$

- (iii) Expressions are derived for the  $\varepsilon_m$ ,  $I_m$ ,  $I_T$  and  $I$  for the effect of post-irradiation deformation on the ML intensity, which are as given below:

$$\varepsilon_m = \frac{1}{(\gamma/\dot{\varepsilon} - D)} \ln \frac{(\chi + \gamma/\dot{\varepsilon})}{(D + \chi)},$$

$$I_m = \frac{\eta n_{FO} r_F \dot{\varepsilon} p_F^0}{b} \exp[-E_a/kT],$$

$$I_T = \frac{\eta n_{FO} r_F \dot{\varepsilon} p_F^0}{b(D + \chi)} \exp[-E_a/kT] \{1 - \exp[-(D + \gamma)\varepsilon]\}$$

and

$$I = \frac{\eta p_F n_{FO} r_F \dot{\epsilon}}{b} \exp[-(D + \chi)\epsilon].$$

- (iv) From the strain dependence of the density of colour centres in deformed crystals, the value of coefficient of deformation bleaching  $D$  is determined and it is found to be 1.93 and 2.00 for KCl and KBr crystals, respectively. The value of  $(D + \chi)$  is determined from the strain dependence of the ML intensity and it is found to be 2.6 and 3.7 for KCl and KBr crystals, respectively. This gives the value of coefficient of deformation generated compatible traps  $\chi$  to be 0.67 and 1.7 for KCl and KBr crystals, respectively.
- (v) So far as strain, temperature, density of colour centres,  $E_a$  and volume dependences are concerned, there exists a correlation between the deformation bleaching and ML in coloured alkali halide crystals.

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