TRAP DEPTHS ANALYSIS OF UNDOPED KCL AND DOPED KCL : SRCL$_2$ SYSTEM

LALIT KUMAR

Department of Physics Meerut College, Meerut (U.P) India lalitksuvaksh@gmail.com

ABSTRACT:

The basic mechanism of Trap depth has been explained and the role of crystal imperfections in observing such an emission has been put forth. The one trapping – one recombination centre model has been discussed along with accompanied first order and second order kinetics. The basic mechanism of TL (Thermo luminescence) has been discussed Finally, the results of trap depth of undoped KCl and Sr^{2+} doped KCl are presented and critically examined.

KEYWORDS: TL, Trap depth, Sr^{2+} doped KCl etc.

I.INTRODUCTION:

The electronic and motional degrees-of-freedom of ions trapped with electromagnetic fields are extremely well decoupled from their environment [1]. Imperfections in a crystal, associated with impurities and /or lattice defects at times create new localized energy levels in the forbidden band gap. The positions of the energy levels depend upon the nature of the imperfections / defects and the host lattice. Some of these defects are capable to trap an electron or a hole and are referred to as electron or hole traps. V_k – centre is also created in an alkali halide crystal due to trapping of a hole. These are described under separate headings as in the following: An anion vacancy has an equivalent positive charge. It can therefore capture an electron to from an F-centre.

F – CENTRE:

The name F – centre is derived from the German word "Farbe", which stands for colour. When the concentration of F- centre is sufficient, the crystal absorbs sufficient light in the visible region in a limited frequency range and as a result the crystal appears coloured. The F-centre is depicted in Fig.1.
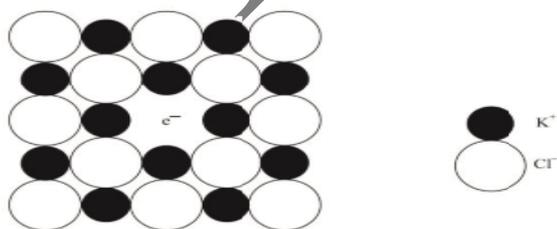

Fig. 1: Two dimensional representation of a KCl crystal showing the F – centre

V$_k$ – CENTRE:

To maintain electro negativity of the crystal , for each electron, which is trapped at an electron trap, a hole is formed. One such hole trap centre is V_k Centre and is shown in Fig. 2. The V_k centre absorbs light in the violet part of the spectrum. This property has led to the naming of such a centre. Actually, a V_k centre is a hole trapped to two neighbouring Cl^- ions in a KCl crystal giving finally a Cl_2^- centre.

THE ONE TRAPPING – ONE RECOMBINATION CENTRE MODEL:

In an ideal crystalline semiconductor or insulator most of the electrons reside in the valence band. The next highest band that the electrons can occupy is the conduction band, separated from the valence band by the so-called forbidden band gap. The energy difference between the delocalized bands is E_g. However, whenever structural defects occur in a crystal, or if there are impurities within the lattice, there is a possibility for electrons to possess energies which are forbidden in the perfect crystal. When a suitable substance is irradiated, electrons are raised from valence band to the conduction band. On return to valence band, some electrons are trapped at some defect locations or trap centres (T), where they can stay for a long time, holes are
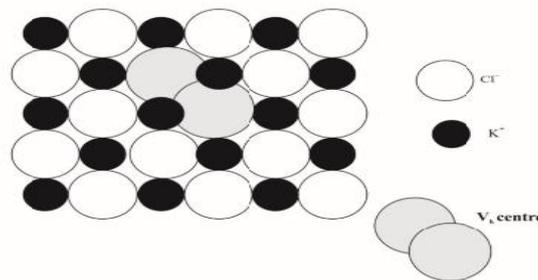

Fig. 2: Two dimensional representation of a KCl crystal showing the V$_k$- centre.

recombination centres (R).The trapped electrons are released from their respective trap centres, when the system is heated[2]. Such released electrons may quickly recombine with an oppositely charged recombination (R) centre, resulting in appearance of a TL glow curve. Let m and n represent the density of holes and electrons in the recombination and trap centres at R and T

respectively. The recombination is the process by which 'm' decreases. Thus the TL intensity, is given by

$$I = -\frac{dm}{dt} = m \, n_c A_m \qquad (1.1)$$

where n_c is the density of electrons in the conduction band and A_m the recombination probability. TL intensity

$$I(t) = -\frac{dm}{dt} \Rightarrow -\frac{dn}{dt} = m n_c A_m$$

$$= \frac{A_m m n s \, e^{-E/kT}}{A_n(N-n) + A_m m}$$

Randall and Wilkins [3, 4] assumed that there is a stronger tendency for electrons to recombine than to get retrapped, i.e.

$$A_m m >> A_n(N-n)$$

Therefore,

$$I(t) = s \, e^{-E/kT} . n$$

and is proportional to first power of 'n' which is obviously time dependant.

SECOND ORDER KINETICS:

Garlic and Gibson [5], however considered the case where retrapping dominates over recombination.

$$A_n(N-n) >> A_m m$$

Then,

$$I(t) = \frac{A_m m}{A_n(N-n)} - n s \, e^{-E/kT}$$

$$= \frac{A_m}{A_n N} s \, e^{-E/kT} . n^2 \quad \text{.......(1.2)}$$

as $m \simeq n$ and $N - n \simeq N$

COLOUR CENTRES AND TL:

The exposure of alkali halides to ionising radiation produces many types of colour centres. The inherent characteristics of such a colouration is that excess electron centres and excess hole centres remain equal. The amount of colouration in an alkali halide to say X-ray exposure is however remains a characteristic of particular alkali halide, purity of sample and its temperature during exposure. The colour centres formed by irradiation can further be transformed into centres of other type by appropriate treatments. Important information about colour centres can be obtained by measuring the changes that occur, when a coloured crystal is gradually heated from some low temperature to a higher temperature. As the temperature of the sample is raised, electrons and holes escape from their traps at an increasing rate. The free charges can recombine with each other or with other defects and often give out luminescence by their recombination.

In practice and in particular in natural minerals, several trapping and recombination sites exist giving rise to a multitude of peaks, which may not overlap.for a general description of the TL process, we need to take into account that the traps show a wide distribution of energy values. In addition we have to take into account several highly relevant processes, including trapping of charge carriers by recombination (luminescence) centres, trapping by non-radiative centers, mutual recombination, recombination's with defects of opposite charges at trapping centers, redistribution of electrons and holes over the available traps and luminescence (re-trapping) due to thermal excitation into the conduction and valence band.

II. EXPERIMENTAL DETAILS:
PREPARATION OF SAMPLES:

The polycrystalline undoped and doped samples of KCl systems, as mentioned were prepared by the saturated solution method. The saturated solution of KCl was prepared in distilled water and one percent by weight of dopant chloride ($SrCl_2$) was added to the mother solution. The resulting liquor was filtered and left for evaporation at 80^0C – 90^0C to yield crystallites of required compounds. These crystallites were reground and pressed in a die to yield appropriate pellets for experiment.

IRRADIATION OF SAMPLES:

The different undoped and doped samples of KCl were irradiated with X-rays of 20mA & 30kV at RT(27^0C) for production of colour centres in them. The exposure time for each sample was kept about the same (900s) for all samples. The irradiated samples were then kept in a blackened container to avoid photo-bleaching of the colour centres.

III. RESULTS AND DISCUSSIONS:
TRAP DEPTH ANALYSIS:

The Randall Wilkins [3] function for the intensity of thermo luminescence at a temperature T, due to a single kind of trap for a monomolecular process, which neglects ret rapping effects is given as,

$$I(T) = n_0 s \exp(-E/kT) \exp$$

$$\left\{-\int_{To}^{T}\frac{s}{\beta}\exp\left(-E/kT'\right)dT'\right\}$$

where, n_0 = total number of trapped charges.

$\quad$ S = a frequency factor.

$\quad$ E = trap depth.

$\quad$ β = dT/dt.

$\quad$ & k = Boltzmann Constant.

The trap depth E and frequency factor s can be determined by fitting the observed glow curves to the above equation while neglecting any temperature variation of s. The simpler formula for first order kinetics as given by Chen [6], however, is

$$E = 0.976\, k\, T_g^2/\delta.$$

where T_g is the glow peak temperature and δ, the half width of glow peak on the fall-off side.

The temperatures corresponding to the maxima of glow peaks and also the corresponding trap depths as estimated from the analysis of the glow peak plots are collated in Table 1. The trap depths were estimated with the help of relation given earlier as

$$E = 0.976\, k\, T_g^2/\delta.$$

IV. CONCLUSION:

The electrons originated due to X-ray irradiation of KCl crystals could be trapped at anion vacancy sites created due to Schottky/Frenkel defects. Such electrons could thus form usual F-centres.

However, if MCl_2 doping is appreciable, as is the case presently with M as Sr, quite a large number of I-V pairs would be created prominently inside a KCl crystal. There is thus a likelihood of electrons being trapped at K^+ sites, close to the vacancy end of I-V pair. With heavy doping of M^{2+}, the second mode of trapping of electrons will be quite probable, as the number of Schottky/Frenkel defects in the KCl crystal will be at a relatively low level. When no

Table.1: The positions of trap depths in undoped and Sr^{2+} - doped KCl

Sample	Trap Depths E(ev)
Undoped KCl (Sample-1)	0.46 ± 0.02
	0.93 ± 0.02
Undoped KCl (Sample-2)	0.44 ± 0.02
	0.95 ± 0.02
KCl : $SrCl_2$	0.78 ± 0.02

external doping is done, a very small number of inherent M^{2+} impurities would always be present in a KCl crystal

and allow electrons to be trapped effectively through both the mechanisms as above.

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