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Trapping Parameter and TL Glow Curve of Ba Doped KCl Crystals

Jagjeet Kaur; Suryanarayana N.S.; Vikas Dubey; P.C. Choubey; Yamini Sahu

Department of Physics, Govt. Vishwanath Yadav Tamaskar Post Graduate Autonomous College, DURG (C.G), 491001, India

> Corresponding author: jsvikasdubey@gmail.com H/P0091 9826937919

Abstract

The present work reports the thermally stimulated luminescence displayed by potassium chloride with different percentages of barium as impurity. The doped KCl:Ba crystal after exposure to UV light is studied. The thermal glow curves exhibited by KCl:Ba shows interesting results. The dependence of dopant concentration on TL in KCl: Ba crystal is investigated. The interaction of ionizing radiations with matter leads to various effects, some of which leave memory in the target material. These memory effects can be seen as the after – effects of the irradiation. This paper describes the sequence of the physical events beginning with the incidence of an ionizing particle, leading to trail of atomic and electronic displacements which stablise in the form of so called defect centres. The kinetics of the thermoluminescence process has been explained phenomenological. The TL phenomenon has found many practical applications. The most outstanding of these are in dosimetry and in archaeology. The paper deals mainly with the physical processes involved in the TL emission and allude briefly to its involvement in applied areas.

Keywords: Computerized glow curve deconvolution, Thermoluminescence, Kinetic Parameters of alkali halide crystals.

1.0 INTRODUCTION:

The study of alkali halides activated by specific impurities is of considerable importance in basic science and technology. The range of application of such studies depends on the nature and concentration of dopant used and also on the type of excitation employed. The analysis of TL glow curves of alkali halide (KCl) due to the variation in concentration level of typical dopant (Ba) is presented in the paper.

Impurities or lattice defects in solids trap unpaired electrons and holes produced in minerals by natural

radiation. The effect of radiation is cumulative and hence the actual amount of the defects can be used in age determination. The defects are metastable and can be released (relaxed), for example by laboratory heating, when the pairs electron/hole are recombined (at characteristic temperatures), that is accompanied by light emission; that is why the process is called thermoluminescence (TL) [1-7]. Thermoluminescence is phosphorescence triggered by temperature above certain point. This should not be confused with incandescence which occurs at high temperatures; in thermo luminescence heat is not the primary source of energy, only the trigger for the release of energy that originally came from another source.

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It may be that all phosphorescence has a minimum temperature; but many have a minimum triggering temperature below normal temperature and are not normally thought of as thermo- luminescence. [8]

Computerized Glow Curve Deconvoluation (CGCD) is not only important but rather essential if one aims to understand the physical processes (i.e. thermal activation of trapped charge (electron/hole) from the traps and its subsequent recombination with its counter part) involving number of parameters depending upon the selected model. Thermoluminescence is a rather complex process involving as many as eight parameters namely activation energy (E), frequency factor (s), recombination probability (A_m) , retrapping probability (A_n) , concentration of the given traps (N), initial concentration in traps (n_0) , intial concentration of holes in centers (m_0) and initial concentration of electrons in the conduction band (n_{c0}) [14]. Retrieving all this parameter is a forbiddable task which has not been achieved for any material. However, the key intrinsic parameters (E, s, A_n, A_m, n₀/N) has been retrieved for some materials like BeO [15], microcline [16] and even glass [17]. CGCD in the present form is used widely in the frame work of general order kinetics formalism [18] which is simple and a practical approach to the problem of deconvoluation. Of course it has own limitation [19-20].

2. Experimental:

Pure and Ba doped KCl crystal were grown by the slow cooling of their melt. The sizes of crystals were taken 2mm^3 before crystals were annealed at 300° C for 1 hour. The UV – radiation was carried out. Crystals of same size were taken and TL output was recorded for measuring the effect of UV dose on TL intensity, the crystals were exposed to different time of UV – radiation.

2.1 Sample Preparation:

The starting materials used for the preparation of the KCl:Ba crystal were KCl powder and Barium Chloride (BaCl₂). The Barium Chloride was added according to the proper ppm and known concentration of dopant Barium was added along with it. This mass was properly crushed and mixed using a mortar and pestle. The mixture so obtained was fired in the central zone of a high temperature muffle furnace at 1000° C for 1 hour. After firing the mixture was then cooled by varying the temperature by 100° C at every hour. The resulting crystal was then effectively cut at known dimensions was used for the study. For UV excitation 365 nm rays obtained from conventional UV sources was used and the different crystals were excited for 40 min and the TL glow curve was recorded with a PC based TL system supplied by Nucleonix with constant heating rate 3.8° C/s.

2.2 Glow curve shape method:

The method based on the shape of glow curve proposed by Chen [18] was used to verify the trapping parameters calculated. The following shape parameters were determined: total half intensity width ($\omega = T_2 - T_1$); the high temperature half width ($\delta = T_2 - T_m$), and; the low temperature half width ($\tau = T_m - T_1$), where T_m is the peak temperature and the T_1 and T_2 are two temperatures on either side of T_m corresponding to half peak intensity. Table 1 shows the different parameter.

2.3 Order of kinetics

The order of kinetics (b) was determined by calculating the symmetry factor (μ) of the glow peak, using the known values of the shape parameters

2.4 Activation energy:

Activation energy (E) was calculated by using the Chen equations, giving the trap depth in terms τ , δ , ω . A general formula for E was given by Chen [18] as follow:

$$\boldsymbol{E} = \frac{C_{y}kT_{m}^{2}}{\gamma} - \boldsymbol{b}_{y}\boldsymbol{2}\boldsymbol{k}\boldsymbol{T}_{m}$$

Fig. 1 shows the Block Diagram of PC based TLD Reader



Fig 1. Block Diagram of PC based TLD Reader

3.0 RESULTS AND DISCUSSION:

Fig 2 represents the variation with TL glow curve as a function of different percentages of Ba. In the recent years thermoluminescence technique has been used as an experimental tool to investigate the nature of luminescence properties of substances including alkali halides. TL is directly related to the band structure of solids and particularly to the effects of the impurities and lattice imperfections. These can be described as defect centers or just centers that may occur when ions of either signs move away from their original sites, thus leaving vacant sites, able to interact with free charge carriers The effect of ionizing radiations like X-rays, on alkali halides doped with divalent and trivalent impurity ions have been studied extensively using this technique [9]. When crystals like alkali halides irradiated with ionizing radiations, electrons and holes are produced and these are generally trapped by the structural defects which are initially present or created by incident ionizing radiations. When the crystal is heated, the electrons or holes will be energized thermally and ejected out of the trap, there is a possibility that they may combine at luminescent centers or recombination centers giving rise to the thermoluminescence. Therefore, the study of thermoluminescence gives the information about the nature of traps, mobile charge carriers and luminescent centers or recombination centers. But the experimental characterization of these materials concerns the parameters such as activation energy, trap depth and the order of kinetics involved in the thermoluminescence process. However, the thermoluminescence occurs due to thermal activation of electrons or due to holes. The thermoluminescence glow peaks occurring at low temperatures can be related to thermal bleaching of Vcentres and F-centres and the glow peaks occurred at above room temperature can be related to F-centres. Elvas et al (1984) found that the mechanoluminescence spectra of gamma irradiated halide crystals consist of a narrow band of different ranges towards the ultraviolet or violet region [10]. S. J. Dhoble et al observed that F centre concentration decreases with decreasing particle size in KCl and KBr [11]. V Ausin *et al* found that the thermoluminescence in irradiated alkali halides is due to the recombination of mobile interstitials with vacancy centres; at some stage in this process light is emitted [12].

In the present investigation the thermoluminescence experiments were made at above room temperature and no impurities were intentionally added to the pure crystal used and therefore it is also expected that Fcentres are involved in the thermoluminescence process. [13]. To analyze the observed TL curves the symmetry factor (µ) [µ = δ / ω , $\delta = T_2 - T_m$, $\omega = T_2 - T_1$, T_m being the peak temperature at the maximum, T_1 and T_2 are respectively, the temperatures on either side of T_m, corresponding to half intensity] is calculated [18]. The peak parameters (peak temperature, full widths, and shape factor) are shown in Table 1. The variation of shape factor (μ) implies that the first peaks is of first order kinetics. Since the shape factor is not unique for the intense peak one can speculate it as a consequence of overlapping of neighboring peaks.

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Fig 2 Thermoluminescence glow curves of Ba doped KCl crystal with 40min UV exposure with the variation of different concentration of Ba

TABLE 1: shape factors (μ) , Activation Energy E and Order of Kinetics b of Ba doped KCl pure crystal and irradiated by UV exposure 365 nm Source

exp time	$ \begin{aligned} \tau &= (T_m - T_1) \end{aligned} $	$\delta = (T_2 - T_m)$	$\omega = (T_2\text{-}T_1)$	$\gamma = \delta \ / \ \tau$	μ= δ/ω	activation energy E eV	Frequency Factor S
pure 40 min	55.24	29.09	84.33	0.52	0.34	0.66	1X10 ⁷
100 ppm 40 min	36.83	18.61	55.44	0.50	0.33	1.06	4.2X10 ⁹
500 ppm 40 min	30.94	17.07	48.01	0.55	0.35	1.29	5.04X10 ¹²

The dependence of shape factor of thermoluminescence (TL) peak exhibiting thermal quenching on the energy (W), characterizing the non radiative process has been thoroughly studied. The shape factor of the first order kinetics is less than 0.4 whereas for a second order kinetics it may be vary from 0.52 to even 0.426 depending on the degree of thermal quenching. This finding gives a caution to the TL workers before reporting general order kinetics without the prior checking of the presence or absence of thermal quenching. [21]

Table 2 The trap depth for the prominent glow peaks of the studied alkali halides, evaluated from first order kinetics

	Activation energy, E (eV)		
Methods	40 mi n pu re	10 0 pp m	50 0 pp m
$E(eV) = T_m(K)/500$	0.5	0.5	0.5
	4	7	7
$E(eV) = 23KT_m$	0.5	0.5	0.5
	4	6	7
$E(eV) = 38KT_m$	0.8	0.9	0.9
	9	3	4
$E(eV) = \frac{2KT_m^2}{\delta}$	0.4	0.7	0.8
	4	5	3
$E_{\omega} = C_{\omega} \frac{KT_{m}^{2}}{\omega} - b_{\omega_{(2K}}T_{m)}$	6.4	0.1	0.2
	2	3	0
$E_{I} = C_{I} (KT_{I} m^{\dagger} 2) / (-b_{I})$	6.7	0.1	0.2
	6	5	1
$E_{I} = C_{I} (T_{T}) (KT_{I}m^{\dagger}2)/(-b_{I})$	7.1	0.1	0.1
	9	1	8

REFERENCES:

[1] Aitken M.J.: *Physics and Archaeology*, Clarendon Press, Oxford 1974.

[2] Daniels et al.: Science 117, 313, 349 (1953).

[3] McKeever: *Thermoluminescence of Solids*, Cambridge University Press, Cambridge 1989.

[4] Fleming S.G.: *Dating in Archaeology*, J.M.Dent & Sons, and London 1976.

[5] Fleming S.G.: *Thermoluminescence Techniques Archaeology*, Clarendon Press, Oxford 1979.

[6] McDougall H.: *Thermoluminescence of geological materials*, Academic Press, London 1968.

[7] Sankaran et al.: Proc.Indian Sci.Acad. 49, 18 (1983).

[8] B.P. Chandra et al.: International Journal of Nanotechnology and Applications Volume 1 Number 2 (2007) pp. 29-34.

[9] G. Baldacchini, O. Goncharova, V.S. Kalinov, R.M. Montereali, A. Vincenti, A.P. Voitovich. Phys. Status Solidi C 4, 1134 2007).

[10] M. Elyas, B. P. Chandra and S. P. Kathuria, Czechoslovak Journal of Physics, Volume 34, Number 2 / February, 1984, 163-168.

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International Journal of Luminescence and Applications Vol.1 (II)

[11] S. J. Dhoble, P. M. Bhujbal N. S. Dhoble and S. V. Moharil, Nuclear

Instruments and methods in Physics research, Volume 192, Issue 3, May 2002, Pages 280-290.

[12] V Ausin et al 1974 J. Phys. C: Solid State Phys. 7 2255-2262.

[13] Meena Laad, *International Journals of Mechanics and Solids*, Volume 4, number 1 (2009), pp. 63-70.

[14] R. Chen and Y.Krish, Analysis of thermally stimulated processes, Pergamon Press, London (1981).

[15] T. Sakurai and R.K. Gartia, J. Phys. D: Appl. Phys. 29 2714 (1996).

[16] T. Sakurai and R.K. Gartia, J. Appl. Phys. 82 5722 (1997).

- [17] T. Sakurai, K. Shoji, K. Itoh and R.K. Gartia, J. Appl. Phys. 89 2208 (2001) .
- [18] R. Chen, J Electrochem. Soc., 116, 1245 (1969).
- [19] T. Sakurai J. Phys. D: Appl. Phys. 34 L105 (2001).
- [20] T. Sakurai and R.K. Gartia, J. Phys. D: Appl. Phys. 36 2719 (2003).

[21] S.Dorendrajit, Singh, "Effect of Thermal Quenching on the shape of a Thermoluminescence glow peak", Luminescence and its Application (1997), pp. 251-255

[22] J.T. Randall and M.H.F. Wilkins, Proc. Roy. Soc. A 184 (1945) 366.

[24] L.I.Lushihik, Soviet Phys. JEPT 3 (1956) 3