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Revisit to power law decay of luminescence

Manish K. Sahai[a,b,*], A.K. Bakshi[a,b], D. Datta[a,b]

[a] Homi Bhabha National Institute, Bhabha Atomic Research Centre, Mumbai 400085, India
[b] Radiological Physics & Advisory Division, Bhabha Atomic Research Centre, Mumbai 400085, India

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ABSTRACT

Luminescence from an exposed sample often follows power-law decay $I \alpha t^{-k}$. I is luminescence intensity, t is time and k is constant. Experimentally range of k is from 0.5 to 2.0. In present study we explain full experimental range of k by considering a non rectangular potential barrier between trap and recombination centre. This study establishes that shape of potential barrier between trap and recombination centre is one of the key factors in explaining power-law decay of luminescence.

1. Introduction

Thermally and optically stimulated luminescence (TL and OSL) are the phenomenon of emission of light as a result of stimulation of material which is previously exposed to ionising radiation. In case of thermoluminescence and optically stimulated luminescence, stimulating agents are heat and light, respectively. During irradiation to ionising radiation, the charge carriers are produced in the material, get trapped at defects centres, and material goes to a metastable state. When material previously exposed to radiation is stimulated by stimulating agent, the trapped charge carriers from metastable states are excited to conduction band/valence band followed by recombination with opposite charge carrier at recombination centres. Recombination leads to release of energy which directly /indirectly produces luminescence. During storage of charge carrier in trap centres, phenomenon of fading occurs. One mechanism of fading is, with time, charge carriers tunnel through the potential barrier to the recombination centres, which may lead to luminescence. Fading due to tunnelling of charge carrier from ground state of the defect centre (trap) to recombination centre is termed as anomalous fading. During the storage period of the exposed material, luminescence light intensity decays with time but the form of decay is not well understood. Generally the decay is observed to follow power-law function, $I \propto t^{-k}$. Where I is the luminescence intensity, t is time and k is a constant. The value of k ranges from 0.5 to 2.0 [1]. The plot of log(I) vs log(st) (note that 's' is frequency factor or attempt-to-escape frequency or pre-exponential factor, which has dimension of time inverse) is observed to be straight line (linear) in many cases, however, in some cases, it was observed to follow non linear behaviour [1]. These observations were reported for storage period ranging from fraction of seconds to much longer periods. [1].

The study of the luminescence signal due to tunnelling is important, particularly in dating applications, because of long storage period of charge carriers in trap is involved, due to prolong exposure period. Due to loss of stored charge carrier, the age of the sample determined through luminescence technique under-estimates the true age of sample. An age correction scheme is possible if the rate of loss of charge carrier in the sample during the storage period is known. Various explanations of fading like defect diffusion [3], radiation less transitions [4] or localised transitions [5] were given, however, the most common explanation for this fading (anomalous fading) is understood to be tunnelling recombination [2].

Literature survey shows that power-law decay of luminescence has been explained only partially [2]. Power-law decay has been explained on the basis of tunnelling of charge carriers from trap to recombination centre, assuming rectangular potential barrier between the two. It was shown that different values of k are obtained for different recombination centre concentrations [2]. However, this approach could explain only values of k ranging from 0.95 to 2.0. For low values of recombination centre concentration, k reaches a lower limit of 0.95. Whereas for high value of recombination centre concentration, poor fit of data (log (I) vs log(st)) to power law function is observed. Till date, although work has been carried out considering rectangular potential barrier between the trap and recombination centre, no explanation was given for considering the same. In fact, defect centres are generally quite complex in nature, and are expected to have complex potential barrier shapes. So it appears rectangular potential barrier in Huntley work [2] was considered only for simplicity. It may be noted that, besides shape of potential barrier, concentration of recombination centre [2], height and width of potential barrier, etc. may also possibly change the value of k.

* Corresponding author at: Homi Bhabha National Institute, Bhabha Atomic Research Centre, Mumbai 400085, India.
E-mail address: mksahai.academic@yahoo.in (M.K. Sahai).

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Present study draws an impact of non rectangular potential barrier between trap and recombination centre. It is tried to establish the fact that shape of potential barrier can also bring in change in the value of k. For this, for a fixed value of recombination centre concentration, full experimental range of k values (0.5–2.0) has been generated computationally by changing shape of potential barrier between trap and recombination centre.

2. Mathematical formulation

In any crystalline material, at microscopic level, there are large but periodic variations in electrostatic potential with change in location. Various models like Kronig Penney model, Muffin Tin potential are adopted [6,7] to explain the periodic variations in electrostatic potential in the crystalline material. These periodic variations in electrostatic potential can be averaged and it can be stated, that macroscopically there is a constant potential which can be fixed as reference level. Rectangular potential barrier can be explained by considering that defects centres (traps/recombination centre) introduce local modifications to the constant potential, mentioned above. In the simplest case, it can be assumed that these modifications by defect centres are finite square wells. In this way, one can explain the rectangular potential barrier between trap and recombination centre. From literature survey [8], it can be established that electrostatic potential close to defect centre is different from what it is at a general location of the crystal. There are many sources of shielded electrostatic potential close to actual defect location due to the presence of foreign atom (e.g dopant). To address this, in the present study, a non rectangular potential barrier (either increasing or decreasing) has been considered, which is not totally random [9].

For mathematical modelling of the phenomena, tunnelling of charge carriers has been modelled with a non rectangular isotropic potential barrier between trap and recombination centre. This is explained in Fig. 1 as region I, II and III. Where a trap is considered to be the region I, region between trap and recombination centre is considered as tunnelling region (region II) and a recombination centre is modelled as region III. Tunnelling phenomena has been presented in three dimensions with isotropic potential. In the model a sphere has been considered in which recombination centres are distributed randomly around a trap. Consequently, to determine the wave function in these three regions, Schrödinger equation in spherical polar coordinate has been considered. Schrödinger equation in all the three regions has the form given in Eq. (1)

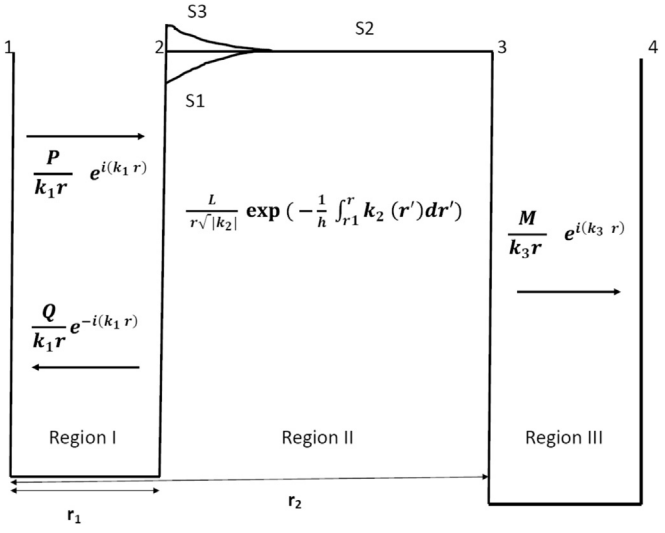

Fig. 1. Schematic representation of different regions: Figure indicates the three regions (I,II and III) with wave functions in them and their boundaries (1, 2, 3 and 4). Region I is trap and Region III is recombination centre. Potential barrier between trap and recombination centre, namely S1 (increasing), S2 (rectangular) and S3 (decreasing) are indicated. Location of boundary 2 is r_1 and of 3 is r_2.

$$\frac{-\hbar^2}{2M}\nabla^2 \ \Psi(r,\theta,\Phi) + V(r)\Psi(r,\theta,\Phi) = E\Psi(r,\theta,\Phi) \tag{1}$$

where

$\Psi(r,\theta,\Phi)$ = Wave function of charge carrier
(r,θ,Φ) = Radial and angular coordinates
$V(r)$ = Potential barrier
E = Energy of charge carrier
M = mass of charge carrier
$\hbar$ = = Plank's constant divided by 2 Π.

The spherical approximation allows us to write $\Psi(r,\theta,\Phi) = R(r)Y_{lm}(\theta,\Phi)$, where $R(r)$ is the radial function, r is the distance of the charge carrier (electron) from centre of the trap and $Y_{lm}(\theta,\Phi)$ are spherical harmonics. Using $rR(r) = \chi$ we can write

$$\Rightarrow \quad \frac{d^2\chi}{dr^2} + \frac{2M}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2Mr^2}\right]\chi = 0 \tag{2}$$

In present case, V(r) is not a constant because we have proposed a non rectangular potential barrier. Besides, it has to satisfy following requirements (i) it should generate required (increasing and decreasing) potential barrier shape for different values of parameters involved as shown in Fig. 2, (ii) the integration which is required to be carried out at a later stage should be possible numerically and (iii) the potential should not be varying very fast so that WKB (Wentzel-Kramers-Brillouin) approximation could be applicable. A reasonable choice of V(r) is therefore

$$\mathrm{V(r)} = \begin{cases} -V_1 & \textit{Region I} \\ V_2 = C_0 + D_0 r^b & \textit{Region II} \\ -V_3 & \textit{Region III} \end{cases}$$

C_0 is a constant whereas D_0 and b are parameters. **'r' is radial distance from trap centre.**

Boundary conditions are $\chi \to 0$ as $r \to 0, +\ \infty$.

Solving Eq. (2) in the three regions we get ground state radial wave functions as

$$\text{Region I}: R_I(k_1 r) = \frac{P}{k_1 r}e^{i(k_1 r)} + \frac{Q}{k_1 r}e^{-i(k_1 r)} \tag{3a}$$

$$\text{Region II}: R_{II}(k_2 r) = \frac{L}{r\sqrt{|k_2|}} \quad \exp\left(-\frac{1}{h}\int_{r1}^{r} k_2(r')dr'\right) \tag{3b}$$

$$\text{Region III}: R_{III}(k_3 r) = \frac{N}{k_3 r}e^{i(k_3 r)} \tag{3c}$$

where k_1, k_3 are the wave vectors corresponding to regions I and III respectively. In region between the trap and recombination centre, the wave vector cannot be defined properly as the height of barrier is function of radial distance, r, but $\frac{k_2}{\hbar}$ has dimension of wave vector for region II. P, Q, L and N are constants.

Both transmission and reflections of wave function can take place at a boundary between two regions. Reflections from boundary 3 of region II and boundary 4 of region III are neglected to make the problem simpler considering the fact that due to multiple reflections, amplitudes of wave function would be relatively small. Further, we apply continuity of wave function and its derivatives at the boundaries 2 and 3. Boundaries are numbered in Fig. 1.

$$R_I(r_1) = R_{II}(r_1) \tag{4a}$$

$$R_{II}(r_2) = R_{III}(r_2) \tag{4b}$$

$$\frac{dR_I}{dr}|_{r=r_1} = \frac{dR_{II}}{dr}|_{r=r_1} \tag{4c}$$