# Evaluation of activation energies in the semi-localized transition model of thermoluminescence

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## Abstract

Recently a semi-localized transition (SLT) kinetic model was developed for thermoluminescence (TL), which is believed to be applicable to important dosimetric materials like LiF : Mg,Ti. This model contains characteristics of both a localized transition model and a single trap model and is characterized by two distinct activation energy levels. This paper describes the simulation of several standard methods of analysis for the TL peaks calculated using the SLT model in an effort to extract the two activation energy parameters of the model. The methods of analysis are applied to both possible types of transitions within the model, namely the direct recombination of the hole–electron pairs as well as the delocalized transitions involving the conduction band. In the former case of direct recombination, the methods of analysis give consistent results for the activation energy $E$. In the latter case of transitions involving the conduction band, it was found that extra caution must be exercised when applying standard methods of analysis to the SLT model because of the possibility of strongly overlapping TL peaks. Specifically the peak shape methods consistently fail to yield the correct value of $E$, while careful application of the fractional glow, thermal cleaning and variable heating rate methods can yield the correct energy values when no retrapping is present within the localized energy levels. A possible explanation is given for the previously reported failure of the peak shape methods to yield the correct activation energies within the SLT model. The heating rate methods of analysis consistently yield the correct activation energies $E$ with an accuracy of a few per cent.

## 1. Introduction

Theoretical models of thermoluminescence (TL) are usually based on the assumption of a uniform spatial distribution of traps (T) and recombination centres (RCs), resulting in models known as the single trap model (STM). On the other hand, several alternative models of TL are based on the existence of electron–hole pairs trapped close to each other and are the basis of localized transition (LT) models.

Several models based on the spatial correlation of T and RCs were proposed in the literature, and calculations within these models were carried out by using Monte Carlo techniques [1–3]. These calculations showed the existence of unusual TL glow curves, in which the main TL peak is occasionally accompanied by a smaller peak called the displacement peak [4, 5]. These models are of practical importance in dosimetric materials like the popular LiF : Mg,Ti in which the peak 5a is believed to be related to LTs, while the main dosimetric peak 5 relates to carriers that escaped from the electron–hole pair system [6, 7].

In a recent paper in this journal Mandowski [8] developed a complex kinetic model for such spatially correlated TL systems, which contains elements from both the LT and STM models of TL. The complexity of this semi-localized

transition (SLT) model is partly due to the presence of two distinct activation energies, $E$ and $E_V$.

There are two possible recombination transitions within the model, leading to two TL peaks denoted in the rest of this paper by $L_B$ and $L_C$. The $L_B$ peak corresponds to the intra-pair luminescence owing to LTs, and the $L_C$ peak corresponds to delocalized transitions involving the conduction band. Mandowski [8] found that for certain parameters in the model, the $L_C$ peak can exhibit non-typical double-peak structure that resembles the TL displacement peaks previously found in spatially correlated systems by Monte Carlo simulations [4, 5].

This double-peak structure of the $L_C$ peaks was interpreted as follows: the first $L_C$ peak corresponds to an increasing concentration of charges accumulating in the excited local level and undergoing intra-pair recombination. The second $L_C$ peak was interpreted as relating to carriers wandering in the crystal, and undergoing recombination with holes in the RC via the conduction band.

The results of Mandowski [8] showed that when no retrapping occurs within the T–RC pair (retrapping ratio $r = 0$), the model produces a single $L_C$ peak with no apparent double-peak structure. When retrapping is present (values of retrapping ratio ranging from $r = 1$ to $r = 100$), the $L_C$ peaks exhibit a double-peak structure.

Mandowski [8] also found that the amount of recombination within the energy level describing the electron–hole pair also influences the shape and relative size of the delocalized peaks. He also studied the effect of the energy gap $E_V$ on the double-peak structure of the $L_C$ peak.

The purpose of this paper is to perform a detailed study of the double-peak structure of the $L_C$ peak, and to ascertain whether it is possible to extract the activation energies $E$ and $E_V$ of the SLT model by applying the usual methods of TL analysis to the $L_C$ peaks. An additional goal of this paper is to investigate whether a double-peak structure is also present in the case of $L_C$ peaks corresponding to no retrapping ($r = 0$). By applying a variety of methods of kinetic analysis it is shown that this is indeed the case.

## 2. The semi-localized transition model

The energy diagram for the SLT model is shown in figure 1(a), together with the possible electronic transitions. Since some of the transitions shown in figure 1(a) depend on the instantaneous number of carriers occupying T and RCs, it is not possible to write kinetic equations using global concentrations of charge carriers in each level. In order to overcome this difficulty, Mandowski [8] introduced the following notation to denote the occupation of all states in a single T–RC unit,

$$\begin{Bmatrix} \bar{n}_e \\ \bar{n} \\ \bar{h} \end{Bmatrix}, \tag{1}$$

where $\bar{n}_e =$ number of electrons in the local excited level, $\bar{n}$ is the number of electrons in the trap level T and $\bar{h}$ is the number of holes in the RC.
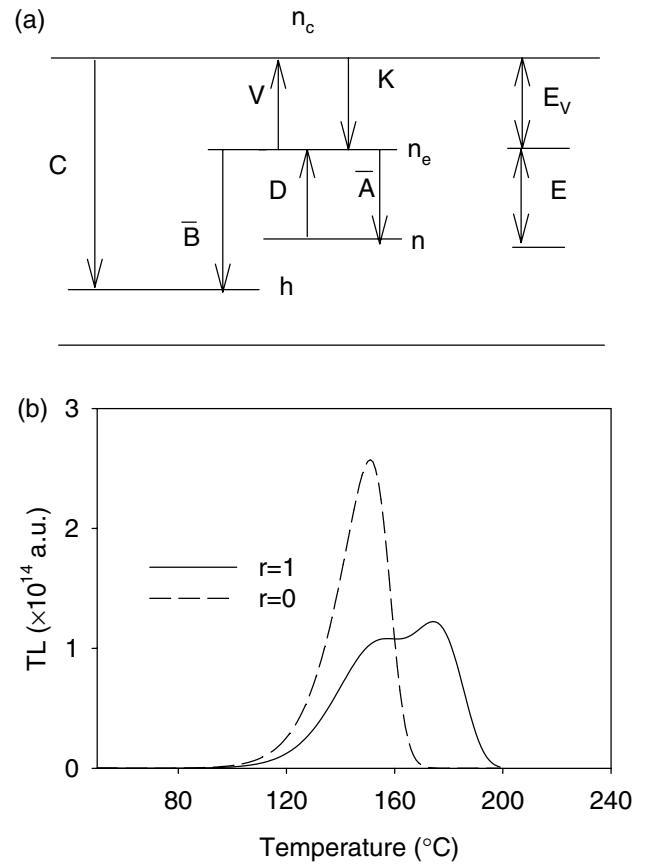
**Figure 1.** (a) The energy levels and transitions of the SLT model. (b) Examples of two $L_C$ peaks produced by the SLT model for $r = 0$ and $r = 1$. The kinetic parameters are given in the text.

By using this notation, the following concentrations of states can be defined,

$$H_0^0 = \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix}, \qquad H_1^0 = \begin{Bmatrix} 0 \\ 1 \\ 1 \end{Bmatrix},$$

$$H_0^1 = \begin{Bmatrix} 1 \\ 0 \\ 1 \end{Bmatrix}, \qquad H_1^1 = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix},$$

$$E_0^0 = \begin{Bmatrix} 0 \\ 0 \\ 0 \end{Bmatrix}, \qquad E_1^0 = \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix},$$

$$E_0^1 = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}, \qquad E_1^1 = \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix}, \tag{2}$$

where $H_m^n(t)$, $E_m^n(t)$ are the concentrations of states with full and empty RCs, respectively.

Mandowski [8] introduced the following simplifying assumptions in the SLT model:

(a) The $K$-transitions shown in figure 1(a) are such that $K = 0$.
(b) The creation of states with two active electrons ($H_1^1$ and $E_1^1$) is unlikely. As a result of this assumption, the model does not contain differential equations for $H_1^1$ and $E_1^1$.
(c) Only $H_1^0$ states are generated initially.

By using the variables $H_m^n(t)$, $E_m^n(t)$ the following set of seven equations was obtained:

$$\dot{H}_1^0 = -(D + Cn_c)H_1^0 + \bar{A}H_0^1, \tag{3}$$

$$\dot{H}_0^1 = DH_1^0 - (\bar{A} + \bar{B} + V + Cn_c)H_0^1, \tag{4}$$

$$\dot{H}_0^0 = VH_0^1 - Cn_cH_0^0, \tag{5}$$

$$\dot{E}_1^0 = Cn_cH_1^0 - DE_1^0 + \bar{A}E_0^1, \tag{6}$$

$$\dot{E}_0^1 = Cn_cH_0^1 + DE_1^0 - (\bar{A} + V)E_0^1, \tag{7}$$

$$\dot{E}_0^0 = \bar{B}H_0^1 + Cn_cH_0^0 + VE_0^1, \tag{8}$$

$$\dot{n}_c = -Cn_c(H_1^0 + H_0^1 + H_0^0) + V(H_0^1 + E_0^1). \tag{9}$$

The parameters in these equations and the corresponding electronic transitions are shown in figure 1(a). The activation energy within the T–RC pair is denoted by $E$, the energy barrier is $E_V$, and the corresponding frequency factors are $\nu$ and $\nu_V$. A linear heating rate $\beta$ is assumed, the recombination coefficients $C$ (cm$^3$ s$^{-1}$) and $\bar{B}$ (s$^{-1}$) are as shown in figure 1(a), and the retrapping coefficient $r$ is defined as $r \equiv \bar{A}/\bar{B}$. In addition to these parameters, the global concentration of traps in the crystal is denoted by $N$ (cm$^{-3}$). The parameters $D(t) = \nu \exp(-E/kT(t))$ and $V(t) = \nu_V \exp(-E_V/kT(t))$ describe the thermal excitation probabilities in the SLT model.

The variables $H_m^n(t)$, $E_m^n(t)$ are related to the standard global variables used in the LT model and the STM of TL is described by the following equations:

$$n = H_1^0 + E_1^0, \tag{10}$$

$$n_e = H_0^1 + E_0^1, \tag{11}$$

$$n_c = H_0^0 - E_0^1 - E_1^0, \tag{12}$$

$$h = H_1^0 + H_0^1 + H_0^0. \tag{13}$$

Here $n$, $n_e$, $n_c$ and $h$ denote as usual the concentrations of carriers in the trap level, excited level, conduction band and RC, respectively.

The system of seven 'stiff' differential equations (3)–(9) was solved by using the differential equation solver in the commercial program *Mathematica*. The typical CPU time for solving this system of equations on a desktop computer and for producing graphs of $H_m^n(T)$, $E_m^n(T)$, $n(T)$, $n_e(T)$, $n_c(T)$, $h(T)$ as a function of temperature was 1–2 min.

The two recombination transitions within the model lead to two possible TL peaks, $L_B$ and $L_C$. The corresponding TL intensities for peaks $L_B$ and $L_C$ are given by:

$$L_B = \bar{B}H_0^1, \tag{14}$$

$$L_C = Cn_ch = Cn_c(H_1^0 + H_0^1 + H_0^0). \tag{15}$$

Figure 1(b) shows an example of $L_C$ peaks calculated by Mandowski [8] for two values of the recombination ratio $r \equiv \bar{A}/\bar{B}$ ($r = 0$ and 1). The rest of the parameters used in the model are: $E = 0.9$ eV, $\nu = \nu_V = 10^{10}$ s$^{-1}$, $\beta = 1$ K s$^{-1}$, $C = 10^{-10}$ cm$^3$ s$^{-1}$, $\bar{B} = 10^3$ s$^{-1}$, $K = 0$, $E_V = 0.7$ eV. The initial concentration of trapped carriers is assumed to be $H_1^0(0) = n_0$ and all other initial concentrations $H_m^n(0)$, $E_m^n(0)$ are assumed to be zero. Furthermore, it is assumed that all states are initially full so that $n_0 = N$, where $N = 10^{17}$ cm$^{-3}$ is the global concentration of traps in the crystal.

The results of figure 1(b) show that for $r = 0$, i.e. when no retrapping occurs within the T–RC pair, the model produces a single $L_C$ peak with no apparent double-peak structure. When
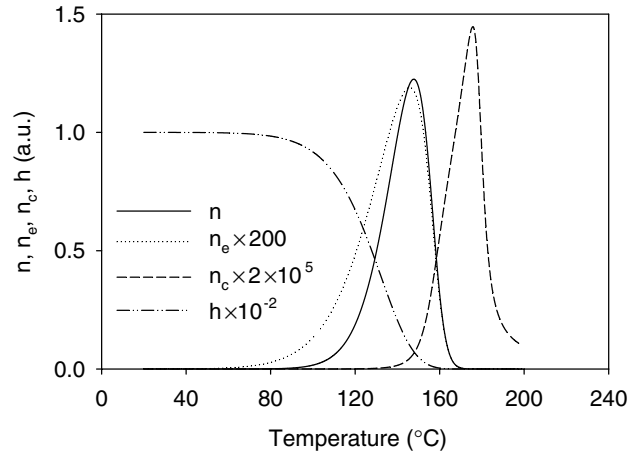


**Figure 2.** The detailed $n$, $n_e$, $n_c$, $h(T)$ graphs for a specific set of parameters given in the text.

values of $r$, between $r = 1$ and 100, are used in the model the $L_C$ peaks have a clear double-peak structure. The methods of kinetic analysis employed in the next section show that an underlying double-peak structure is also present in the case of the $L_C$ peak corresponding to $r = 0$.

Figure 2 illustrates the detailed variation of the concentrations $n(T)$, $n_e(T)$, $n_c(T)$, $h(T)$ with temperature during heating of the material from room temperature to 200°C, producing the single $L_C$ peak shown in figure 1(b) for $r = 0$.

The next section demonstrates how the two distinct activation energies $E$ and $E_V$ can be extracted from TL glow curves calculated within the SLT model.

## 3. Simulation of methods of kinetic analysis—numerical results

A variety of methods of kinetic analysis were used to analyse the $L_B$ and $L_C$ peaks of the SLT model for the case of no retrapping ($r = 0$), as well as for cases with high retrapping ($r = 1$–100). Owing to the complexity of the SLT model, one might expect that the methods of analysis will yield different results from the well-studied STM and LT models, and the results show that this is indeed the case.

In section 3.1 we present the results of applying the peak shape and heating rate methods of analysis to the single-peak $L_B$ glow curves of the SLT model, for values of the recombination ratio $r$ between $r = 0$ and 100. The results show that in all cases the $L_B$ peaks follow first order kinetics.

In section 3.2 the heating rate methods of analysis are applied to the double-peak $L_C$ glow curves of the SLT model, when significant retrapping is present ($r = 1$–100). It is found that the heating rate methods in these cases yield the correct values for the two distinct activation energies $E$ and $E_V$ of the SLT model, with an accuracy of a few per cent.

It is also found that the heating rate method fails to yield the correct energy in the case $r = 0$, i.e. when no retrapping is present within the T–RC pair. Since the $L_C$ peak for $r = 0$ shows no discernible double-peak structure (figure 1(b)), it is possible that this failure of the heating rate method may be

**Table 1.** Summary of kinetic analysis of single-peak $L_B$ glow curves.

| $r$ | $E$ (eV) from heating rate method | | $E$ (eV) from peak fitting method | | FOM of fitting method |
|-----|------|-------|------|--------|-------|
| 0   | 0.93 | (+3.3%) | 0.90 | (0%) | 0.025 |
| 1   | 0.92 | (+2.2%) | 0.91 | (+1.1%) | 0.015 |
| 10  | 0.90 | (0%) | 0.96 | (+6.7%) | 0.026 |
| 100 | 0.96 | (+6.7%) | 1.02 | (13.3%) | 0.037 |

The numbers in parentheses indicate the per cent difference from the expected value of $E = 0.9$ eV for transitions within the T–RC pair.
The accuracy of the $E$-values shown in all cases is $\pm 0.01$ eV.
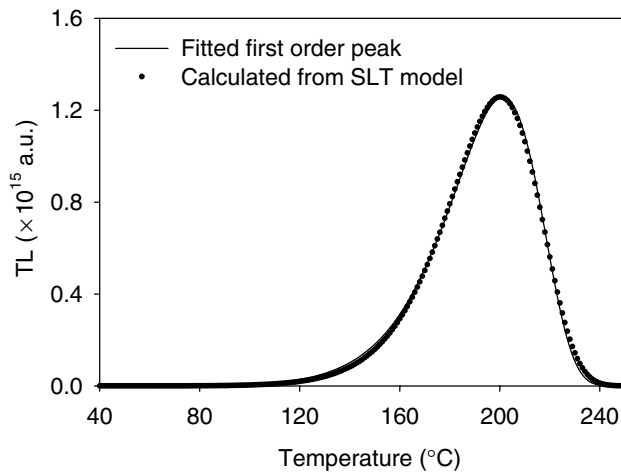


**Figure 3.** Results of first order peak fitting analysis of the $L_B$ glow curve for $r = 100$. Similar accurate fits were obtained for all values of the recombination ratio $r$.

due to the existence of an underlying double-peak structure in the $L_C$ peak. This is shown to be the case in section 3.3, where the double-peak structure is revealed by simulating the fractional glow method of analysis.

Finally in section 3.4 we apply the peak-shape methods of analysis to the $L_C$ peaks and find that these methods systematically fail to yield the correct activation energies $E$ and $E_V$. A possible explanation for this failure is given by examining the concentration of electrons in the conduction band $n_c(T)$ at various temperatures.

### 3.1. Analysis of $L_B$ peaks in the SLT model for r = 0–100

From previously published theoretical analysis of the LT model [9], we might expect that the $L_B$ peaks in the SLT model will follow first order kinetics even in cases of strong recombination within the trap level. The results of applying various standard methods of analysis to the $L_B$ peaks are shown in table 1. Excellent fits are obtained by fitting the $L_B$ peaks with first order kinetics expressions, for values of the retrapping ratio $r$ between $r = 0$ and 100. Table 1 contains the values of figure of merit (FOM) obtained by these first order fits. The FOM values vary from 0.025 to 0.037 (i.e. 2.5–3.7%) when $r$ varies from $r = 0$ to 100.
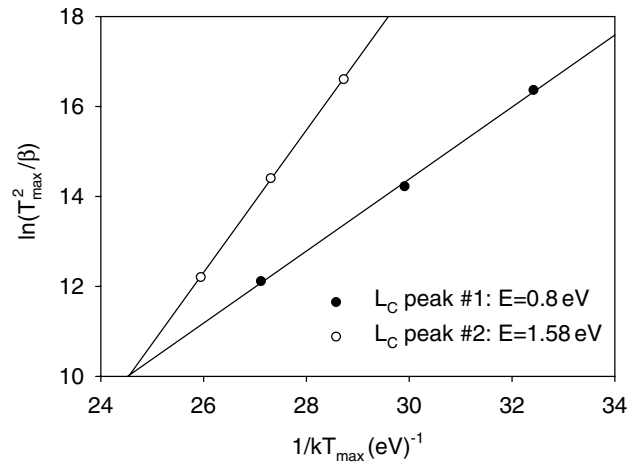
**Figure 4.** Results of applying the variable heating rate method for the two apparent peaks in the $L_C$ glow peak for $r = 1$. The correct values of the energy $E = 0.9$ and $E + E_V = 1.6$ eV are obtained from the slope of the graphs. When $r = 0$ the method yields the incorrect value of $E = 1.07$ eV because of the underlying double-peak structure.

The accuracy of the calculated values of the activation energy $E$ from the first order fitting procedure ranges from an error of 0% (for $r = 0$) to the worst case error of 13% (for $r = 100$). A typical first order fit is shown in figure 3 for the case $r = 100$. It must be noted that cases of very high recombination ratios $r$ (such as the case $r = 100$) are of purely theoretical interest, since glow peaks corresponding to such high values of the recombination ratio have not been observed experimentally so far in TL materials.

By applying the well-known heating rate method of analysis to the $L_B$ peaks, one also obtains the correct values for $E = 0.9$ eV (in our examples, within 5% or better). In these well-known techniques, the TL glow curves are measured with different heating rates $\beta$ and the temperatures $T_{max}$ of maximum TL intensity are recorded. A graph of $\log(T_{max}^2/\beta)$ versus $1/kT_{max}$ yields a straight line of slope equal to the activation energy $E$. These results are also shown in table 1, indicating close agreement between the heating rate and peak shape methods of analysis for the single-peak $L_B$ glow curves, for values of $r$ between $r = 0$–100.

### 3.2. Analysis of $L_C$ peaks in the SLT model using the heating rate methods

In simulating the heating rate method of TL analysis, the heating rate was varied within a typical experimental range of 0.01–20 K s$^{-1}$. No double-peak structure was discernible in any of these heating rates for the case $r = 0$, while a clear double-peak structure was obvious for $r = 1, 10, 100$.

The results of applying the heating rate method to the two $L_C$ peaks for $r = 1$ are shown in figure 4, and the corresponding energy values are summarized in table 2 for all values of $r$ between $r = 0$ to 100. The data in table 2 show that in all cases where $r \neq 0$ the heating rate method produces the correct values for the two activation energies in the SLT model $E_1 = E = 0.9$ eV and $E_2 = E + E_V = 1.6$ eV with an accuracy of 3–11%.

**Table 2.** Summary of kinetic analysis of the $L_C$ glow curves using the heating rate method.

| $r$ | $L_C$ peak 1 $E$ (eV) from heating rate method | | $L_C$ peak 2 $E$ (eV) from heating rate method | |
|---|---|---|---|---|
| 0 | 1.07 | (+18.9%) | — | (single-peak is assumed) |
| 1 | 0.80 | (−11.1%) | 1.58 | (−1.3%) |
| 10 | 0.92 | (+2.2%) | 1.60 | (0%) |
| 100 | 0.87 | (−3.3%) | 1.64 | (+2.5%) |

The numbers in parentheses indicate the per cent difference from the expected values of $E = 0.9\,\text{eV}$ and $E + E_V = 0.9 + 0.7 = 1.6\,\text{eV}$ for delocalized transitions involving the conduction band.

The heating rate method for $r = 0$ gave a high activation energy $E = 1.07\,\text{eV}$, which is 19% higher than the expected value of $E = 0.9\,\text{eV}$. The most probable explanation for this failure of the heating rate method for $r = 0$ is the existence of an underlying double-peak structure. This hypothesis is investigated in some detail in the following section.

### 3.3. Analysis of $L_C$ peaks in the SLT model for $r = 0$

In order to investigate the possibility of a multiple-peak structure of the $L_C$ peak in the case $r = 0$, we simulated three common experimental variations of the initial rise (IR) and fractional glow (FG) methods, which are based on the use of either a single aliquot or multiple aliquots of the sample [9, 10]. These three variations of the experimental technique yield different results for the activation energies, illustrating the complexity of the SLT model and the need for careful analysis of the $L_C$ peaks within this model.

The details of the three variations of the FG method are as follows, and the results of the simulations are shown in figures 5–8.

*3.3.1. Single-aliquot IR method.* In this method a single aliquot of the material is heated up to a temperature $T_{stop}$ located well below the maximum of the TL glow curve, and is subsequently cooled to room temperature. The process is then repeated several times by heating the same aliquot to a slightly higher temperature each time, to yield the partial glow curves in figure 5(b). The heating procedure for this method is shown schematically in figure 5(a).

By performing an IR analysis of the curves in figure 5(b) obtained in this fashion, the activation energy $E$ is calculated for each temperature $T_{stop}$. A 'staircase' graph of $E$ as a function of $T_{stop}$ indicates the presence of several distinct activation levels $E$ [10].

The results of simulating this experimental method are shown in figure 5(c) which indicate the presence of two TL peaks with energies $E_1 = 1.6\,\text{eV}$ and $E_2 = 0.9\,\text{eV}$. The value of $E_2$ corresponds to the activation energy $E$ within the T–RC pair, and the value of $E_1$ corresponds to the total energy $E_1 = E + E_V$ required for the electrons to be raised to the conduction band. A rather unusual feature of the 'staircase' energy structure shown in figure 5(c) is the fact that while, one usually expects an ascending staircase structure, the data in figure 5(c) clearly show a 'descending' staircase structure.
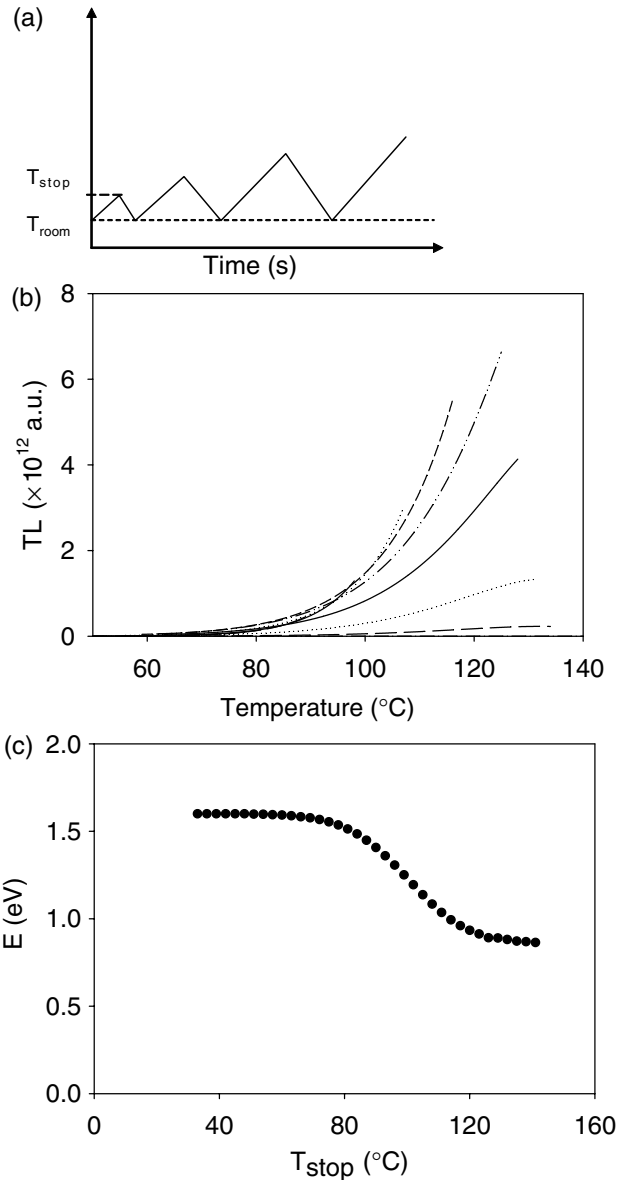


**Figure 5.** (a) The heating procedure employed in the single-aliquot IR method of analysis. (b) The partial glow curves obtained when applying the heating process in (a). (c) The staircase structure of the $E$–$T_{stop}$ graph reveals the presence of a double-peak structure with the correct values of the energy $E = 0.8\,\text{eV}$ and $E + E_V = 1.6\,\text{eV}$.

This unexpected result was verified by simulating the multiple aliquot method of analysis as described below.

*3.3.2. Multiple aliquot IR method.* In this method an aliquot of the material is heated up to a temperature $T_{stop}$ well below the maximum of the TL glow curve, and is subsequently cooled to room temperature. Immediately after, the aliquot is heated all the way to a high temperature (e.g. 200°C) and the remaining TL glow curve is obtained. The process is then repeated several times by heating a different aliquot to a slightly higher temperature $T_{stop}$ each time. The heating procedure for this method is shown schematically in figure 6(a).

This method produces a series of TL glow curves, essentially corresponding to a thermal cleaning process of the
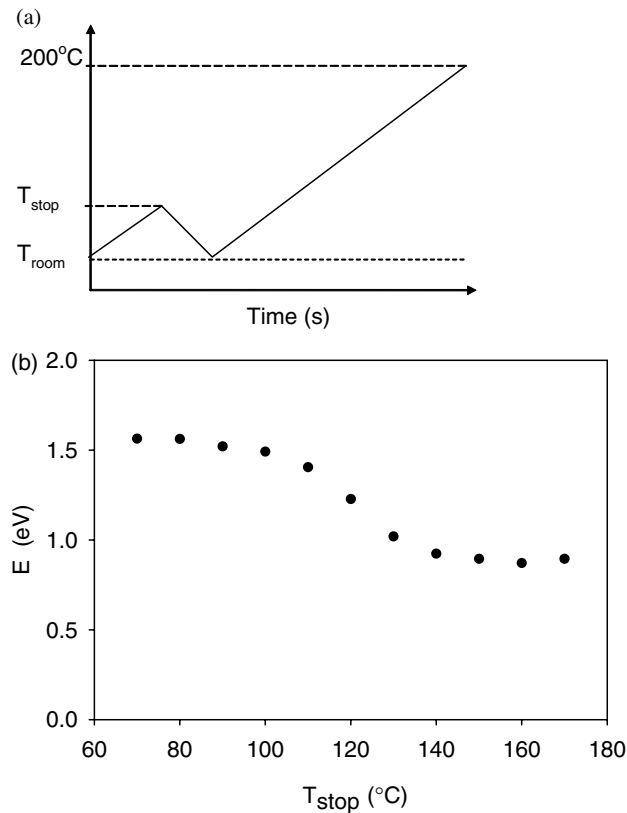
**Figure 6.** (*a*) The heating procedure employed in the multiple-aliquot $T_{max}$–$T_{stop}$ method of analysis. (*b*) The structure of the $E$–$T_{stop}$ graph obtained by IR analysis of the TL glow curves when using the heating scheme shown in (*a*).

TL glow curve. By performing an IR analysis of the TL glow curves obtained in this fashion, the activation energy $E$ is calculated for each temperature $T_{stop}$.

It is noted that in this method both a $E$–$T_{stop}$ graph and a $T_{max}$–$T_{stop}$ graph are obtained, and a series of TL glow curves is produced. The results of simulating this experimental method are shown in figure 6(*b*) where a 'descending staircase' $E$–$T_{stop}$ structure is found again, consistent with the data in figure 5(*c*). The corresponding glow curves are shown in figure 7(*a*) and the additional 'staircase' $T_{max}$–$T_{stop}$ graph is shown in figure 7(*b*).

A closer look at the TL glow curves shown in figure 7(*a*) indicates that as the material is heated towards progressively higher temperatures $T_{stop}$, the temperature of maximum TL intensity $T_{max}$ shifts towards smaller temperatures, indicating the presence of strongly overlapping TL peaks with energies $E_1 = E = 0.9$ eV and $E_2 = E + E_V = 1.6$ eV.

These results show that the SLT model involves complex kinetics that can produce unusual results owing to the presence of two activation energies $E$ and $E_V$, and that kinetic analysis of the glow curves in the SLT model should be carried out with the utmost care.

*3.3.3. The FG method of analysis.* In this method of TL analysis an aliquot of the material is heated up to a temperature $T_{stop}$ well below the maximum of the TL glow curve, and is subsequently cooled by a few degrees but not all the way to room temperature. The process is repeated several times by
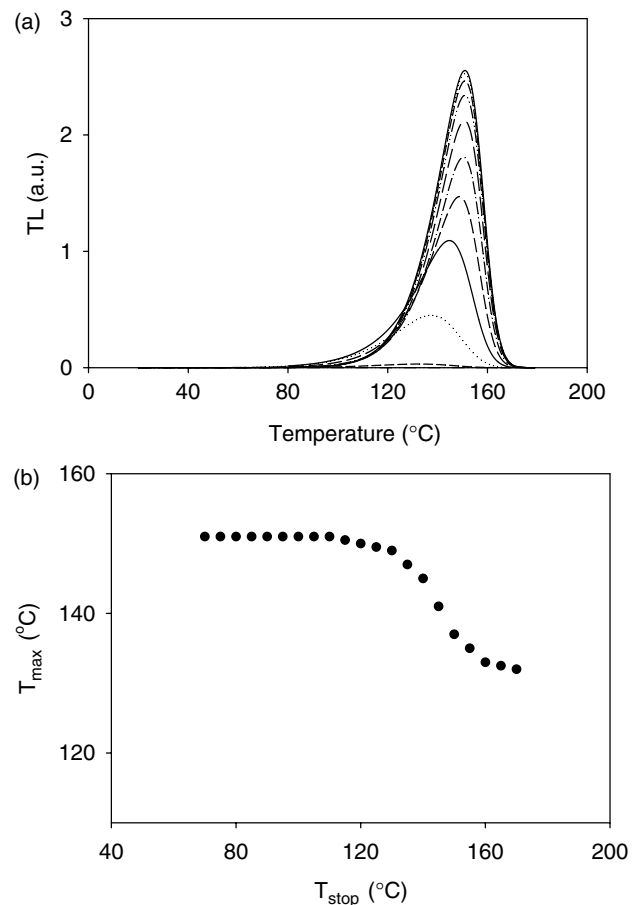
**Figure 7.** (*a*) The TL glow curves obtained by applying the $T_{max}$–$T_{stop}$ method in figure 6. (*b*) The $T_{max}$–$T_{stop}$ analysis yields a staircase structure and an unusual shift of the temperature of maximum TL intensity $T_{max}$ towards lower temperatures.

heating the same aliquot to a slightly higher temperature $T_{stop}$ each time, as shown schematically in figure 8(*a*).

By performing an IR analysis of the descending and ascending curves obtained in this fashion, the activation energy $E$ is calculated for each temperature $T_{stop}$. The results of simulating this experimental method are shown in figure 8(*b*) where surprisingly a 'staircase' structure is not present, but rather a single energy $E = E + E_V = 1.6$ eV is found.

A possible qualitative explanation for this discrepancy between figure 8(*c*) and figures 6(*b*) and 5(*c*) can be seen from the three different heating schemes used in these simulations. In the FG method the sample does not cool down all the way to room temperature, but rather is continuously heated to higher temperatures in small steps. The presence of progressively higher temperatures causes continuous direct excitation of the electrons into the conduction band according to the Boltzmann factor $\exp(-(E+E_V)/kT)$, and hence this method of analysis yields only the total activation energy $E + E_V = 1.6$ eV.

*3.4. Peak-shape methods for the $L_C$ peaks*

Mandowski [8] attempted to fit the intensity of the delocalized transitions $L_C$ with two first order TL peaks. His results indicated that the two-peak analysis for any value of $r$ leads in general to very high values of the activation energy $E$.
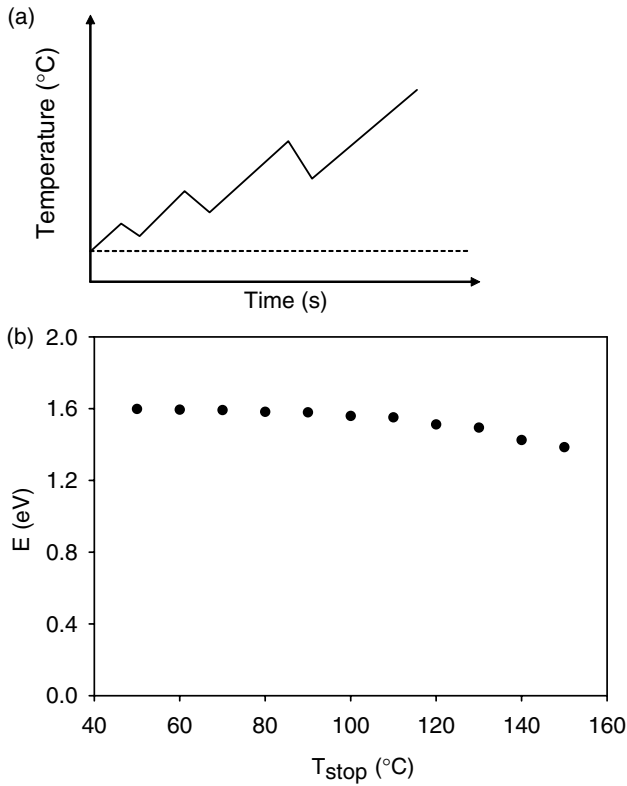
**Figure 8.** (*a*) The heating procedure employed in the single-aliquot FG method of analysis. (*b*) The FG method yields a single *E*-value of $E + E_V = 1.6\,\text{eV}$.

For example, in the case $r = 0$, $E = 0.9\,\text{eV}$ and $E_V = 0.7\,\text{eV}$ studied here, the glow curve deconvolution analysis yielded the values of $E_1 = 1.41\,\text{eV}$ and $E_2 = 2.48\,\text{eV}$ (shown in table 1 of [8]).

Our attempts to fit the $L_C$ glow curves to two first order peaks yielded very good curve fits but led to similar high values of the energy $E$. A possible explanation for the consistently high values of $E$ obtained using peak shape methods in the SLT model is as follows.

It is noted that the temperature dependence of the $L_C$ peak is derived from the two terms $n_c(T)$ and $h(T)$ in equation (15). Figure 9(*a*) shows that the function $\ln(h)$ is almost constant in the temperature interval 20–150°C of the glow peak; therefore, the temperature dependence of the $L_C$ peak within this temperature interval is determined solely by the faster varying function $\ln(n_c)$.

From a physical point of view, we might expect that as the sample is heated to higher temperatures, the function $n_c(T)$ will increase according to the Boltzmann factor $\exp(-E'/kT)$ where the activation energy $E' = E + E_V$ represents the effective energy required to raise the electrons from the ground state of the trap into the conduction band. Figure 9(*b*) shows that this is indeed the case: a graph of $\ln(n_c)$ versus $1/kT$ yields a straight line of slope $E + E_V = 1.60\,\text{eV}$ in the interval 20–140°C.

This observation provides a plausible explanation for the previously reported failure of the peak shape methods to produce the correct *E*-values, since the $n_c(T)$ term in equation (15) dominates the temperature-dependence of the TL-intensity $L_C(T)$ over a temperature region that clearly
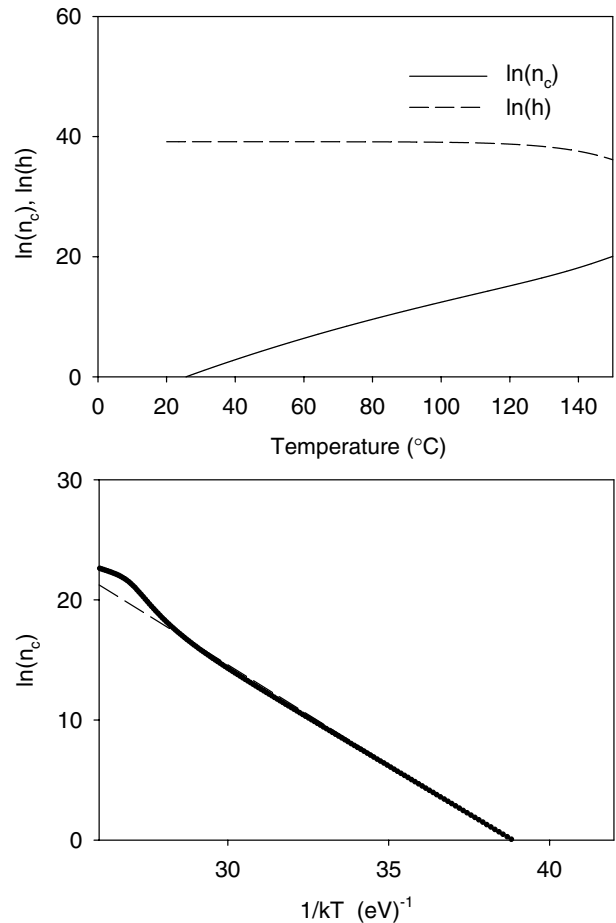


**Figure 9.** (*a*) The temperature variations of the functions $\ln(n_c)$ and $\ln(h)$ in equation (15). (*b*) A graph of $\ln(n_c)$ versus $1/kT$ for the case $r = 0$ yields a best fitted line of slope of $E + E_V = 1.6\,\text{eV}$ over the temperature range of the glow curve (- - - -).

extends over most of the glow peak. As a result of the temperature dependence of the glow curve on the term $n_c(T)$, the peak shape methods are likely to yield high values of the activation energy.

## 4. Conclusions

In this paper a variety of methods of kinetic analysis were used to analyse the $L_B$ and $L_C$ peaks of the SLT model for the case of no retrapping ($r = 0$) as well as for cases with high retrapping ($r = 1–100$). Owing to the complexity of the SLT model, it was found that the methods of analysis yield unusual results, partly due to the presence of two distinct activation energies within the model.

By applying the peak shape and heating rate methods of analysis to the single-peak $L_B$ glow curves of the SLT model it was found that these peaks follow first order kinetics for any value of the recombination ratio $r$ between $r = 0$ and 100.

The heating rate methods of analysis were applied to the double-peak $L_C$ glow curves of the SLT model, when significant retrapping is present ($r = 1–100$). It is found that the heating rate methods in these cases yield the correct values for the two distinct activation energies $E$ and $E_V$ of the SLT model, with an accuracy of a few per cent.

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It is also found that the heating rate method fails to yield the correct energy in the case $r = 0$ owing to the existence of an underlying double-peak structure in the $L_C$ peak. This underlying double-peak structure was revealed by simulating the fractional glow method of analysis.

The peak shape methods of analysis were applied to the $L_C$ peaks and they failed to yield the correct activation energies $E$ and $E_V$. A possible explanation for this failure was given by examining the concentration of electrons in the conduction band $n_c(T)$ at various temperatures. The results of this paper demonstrate the complexity of the SLT model and indicate that further study of the model is necessary with different sets of parameters before the model can be useful in extracting the kinetic parameters from experimental TL glow curves.

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