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New expressions for half life, peak maximum temperature, activation energy and kinetic order of a thermoluminescence glow peak based on the Lambert *W* function

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HIGHLIGHTS

- A new general approximate analytical expression for half life is derived.
- The condition for the maximum in TL is solved over E and T_m based on Lambert *W* function.
- A new analytical expresion for kinetic order versus symmetry factor is derived.
- The new kinetic order analytical expression was verified by simulation.

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ABSTRACT

In this work approximate analytical expressions are derived for four different aspects of Thermoluminescence (TL) kinetics, by using the Lambert *W* function. Firstly, analytical expressions are derived for the half life of trapped charge in a single trap within the one trap one center model (OTOR), and these are compared with analytical equations based on the empirical general order (GO) kinetics. Secondly, approximate analytical expressions are obtained for the temperature T_m of maximum TL intensity in a glow peak and for the activation energy E, by solving the condition for the maximum. Finally, an analytical expression was derived for evaluating the kinetic order b as a function of the integral symmetry factor μ'_g of an experimental TL peak. Where necessary, the analytical expressions were successfully verified by numerical simulations of the OTOR model by using a wide range of possible values of the parameters in this model.

1. Introduction

The one-trap one-recombination center model (OTOR) is the simplest and most fundamental model for luminescence studies. Although various aspects of the model have been studied extensively during the past 50 years, it was only recently that analytical solutions were obtained for this model, by using the well known Lambert *W* function. Kitis and Vlachos (2013) used the transcendental Lambert function to solve the differential equation of the OTOR model, and were able to derive a general analytical equation which can describe any stimulation luminescence mode within the framework of this model.

This paper continues the work by Kitis and Vlachos (2013), and presents several sets of new analytical equations for several aspects of luminescence phenomena within the OTOR model.

The first set of analytical equations concerns the half life $\tau_{1/2}$ of charge loss from a single trap, during optical or thermal stimulation. The half life $\tau_{1/2}$ is one of most important parameters for the correct application of thermoluminescence (TL) or optically stimulated luminescence (OSL) in radiation dosimetry and in luminescence dating. For example, the charge loss during an isothermal thermoluminescence (ITL) experiment is usually assumed to be a single exponential function, and the half life $\tau_{1/2}$ of this process is evaluated by the simple first order kinetics expression:

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$$\tau_{1/2} = \ln 2/\lambda, \tag{1}$$

where $\lambda = s\exp(-E/kT)$ is the probability of thermal excitation. In this equation $s(s^{-1})$ is the frequency factor, $E(eV)$ the activation energy, $k(eV/K)$ is the Boltzmann constant and $T(K)$ is the absolute temperature. However, of more general interest are the lifetimes for non-first order kinetics processes. Some analytical expressions for $\tau_{1/2}$ exist in the literature, which are based on the empirical differential equation for general order (GO) kinetics (Chen and McKeever, 1997; Furetta and Kitis, 2004; Chen and Pagonis, 2015). Also recently an analytical expression for $\tau_{1/2}$ was developed by Lovedy and Gartia (2013a) within the OTOR model.

Section 3 in this paper presents a set of more general analytical expressions for $\tau_{1/2}$ in the OTOR model, during three different types of stimulation modes: an isothermal TL (ITL) process, a continuous wave optically stimulated luminescence process (CW-OSL), and a linearly modulated OSL process (LM-OSL). These analytical equations are compared with analytical equations based on the empirical general order (GO) kinetics and with the analytical expression for ITL derived by Lovedy and Gartia (2013a).

The second set of analytical equations presented here relates to one of the best known equations in thermoluminescence (TL) phenomena, namely the equation for the temperature T_m of maximum intensity in a single TL glow peak (Chen and Kirsh, 1981; Chen and McKeever, 1997):

$$\frac{\beta E}{kT_m^2} = f_{gen} s\exp\left(-\frac{E}{kT_m}\right). \tag{2}$$

where β is the heating rate, and the dimensionless coefficient f_{gen} is a slowly varying function of the parameters in the OTOR model. Within the context of general order (GO) kinetics, the parameter f_{gen} is given by the expression (Chen and McKeever, 1997)):

$$f_{gen} = 1 + (b-1)\frac{2kT_m}{E}. \tag{3}$$

where b is the kinetic order of the TL process. Although Eq. (2) is widely used to analyze experimental TL glow curves, in general it can not be solved analytically either for the activation energy E, or for the temperature of maximum intensity T_m. In Section 4 of this paper analytical expressions are derived for the temperature T_m of maximum TL intensity and for the activation energy E, in terms of the parameters in the OTOR model by using the W function.

The kinetic order b is also an important parameter which is commonly evaluated by using experimental characteristics of a TL glow peak. Approximate analytical expressions for b are given in the literature, which are usually based on the geometrical symmetry factor $\mu_g = \delta/\omega$ (Chen and McKeever, 1997)). Section 4 contains the derivation of a new analytical expression for the kinetic order b, as a function of the experimentally obtained *integral* symmetry factor μ'_g.

Finally Section 5 discusses the new equations and presents numerical simulations of the OTOR model, by using a wide range of possible values of the parameters in this model.

2. Summary of recent work with the Lambert *W* function within the OTOR model

This section summarizes the recently derived analytical equations by Kitis and Vlachos (2013) for the OTOR model, which are based on the W function.

The properties of the Lambert $W-$function have been comprehensively presented by Corless et al. (1996). This function is defined as the inverse of the function $f(z) = ze^z$, satisfying $W(z)e^{W(z)} = z$ for any complex number z. The Lambert $W-$function is a multivalued function displaying infinite complex branches and only two real ones, which are of interest in the present work. The first real branch is defined for $-\frac{1}{e} \le z \le \infty$ and it is denoted by $W[0,z]$, or $W_0[z]$, or simply $W[z]$. The second real branch is defined for $-\frac{1}{e} \le z \le 0$ and it is denoted by $W[-1,z]$ or $W_{-1}[z]$. Valluri et al. (2000) and Barry et al. (2000) presented an extensive list of its applications in various research fields.

The differential equations describing the OTOR model under the approximation of the quasi-equilibrium condition lead to the general one trap (GOT) equation (Chen and McKeever, 1997). Kitis and Vlachos (2013) used the Lambert W function to solve the GOT equation and to derive a general analytical equation which can describe any stimulation luminescence mode within the OTOR model. Similarly, Lovedy and Gartia (2013b) arrived at the results of Kitis and Vlachos (2013) by using the Wright ω function, which is equivalent to the first real branch of the Lambert W function. Due to its importance, the Lambert W function has been implemented as a built-in function in all widely used software packages (Mathematica, MATLAB, MAPLE, GNU scientific library, Origin, Excel etc.). In the software package *Mathematica* used in the present work, this function is implemented as *ProductLog[x]* for the first real branch, and as *ProductLog[-1,x]* for the second real branch.

Kitis and Vlachos (2013) showed that the solution of the GOT equation leads to a transcendental equation of the form:

$$y + \ln(y) = z, \tag{4}$$

with

$$y = \frac{n_0}{nc}, \tag{5}$$

and

$$c = \frac{n_0}{N}\frac{1-R}{R}, \tag{6}$$

where N is the concentration of available electron traps, n and n_0 are instant and initial concentrations of trapped electrons correspondingly, and $R = A_n/A_m$ is the ratio of the retrapping coefficient A_n and the recombination coefficient A_m .

According to Corless et al. (1996) and Kitis and Vlachos (2013), the solution of Eq. (5) is given in terms of the Lambert W function, as

$$y = W_0[e^z]. \tag{7}$$

Kitis and Vlachos (2013) showed that the value of z when $A_n < A_m$ is:

$$z = \frac{1}{c} - \ln(c) + \frac{1}{1-R}\int_0^t p(t')\mathrm{d}t', \tag{8}$$

where $p(t)$ is an expression describing the simulation mode used in the model.

3. Analytical expressions for $\tau_{1/2}$ in the OTOR model

In this section we derive general approximate analytical expressions for the half life $\tau_{1/2}$ of the trapped charge in a single trap, within the framework of OTOR model. Subsection 3.1 presents a derivation of $\tau_{1/2}$ by using the W function, and for three different modes of stimulation. Subsection 3.2 presents an alternative method of deriving the expressions for $\tau_{1/2}$ by using a parametric equation for the OTOR model. The special case of constant thermal excitation is discussed in connection with analytical equations for $\tau_{1/2}$ derived by Lovedy and Gartia (2013a). Subsection 3.3 presents previously derived equations for $\tau_{1/2}$ in the GO model, and these are compared with the analytical expressions for $\tau_{1/2}$ in the OTOR model.

3.1. Derivation of $\tau_{1/2}$ from GOT equation of the OTOR model using the W function

In this subsection we derive an analytical expression for the half life of the trapped charge in a single trap, in the framework of OTOR model. The derivation will be based on the analytical solution of GOT equation of the OTOR model involving the Lambert function. In the next subsection an alternative derivation is given by using parametric equations in the OTOR model.

From Eqs. (5) and (7) we have

$$\frac{n_0}{nc} = W[e^z]. \tag{9}$$

The half life is defined as the time $\tau_{1/2}$ for which $n = n_0/2$. So Eq. (9) gives

$$W[e^z] = \frac{2}{c}. \tag{10}$$

From Eq. (10) and by definition (Corless et al., 1996) z will be:

$$z = \frac{2}{c} + \ln\left(\frac{2}{c}\right). \tag{11}$$

Equating Eq. (11) and Eq. (8) and setting $t = \tau_{1/2}$ we obtain:

$$\frac{2}{c} + \ln\left(\frac{2}{c}\right) = \frac{1}{c} - \ln(c) + \frac{1}{1-R}\int_0^{\tau_{1/2}} p(t')\mathrm{d}t'. \tag{12}$$

After some simple algebra and replacing c from Eq. (6), the following general expression is obtained:

$$\int_0^{\tau_{1/2}} p(t')\mathrm{d}t' = \frac{NR}{n_0} + (1-R)\ln 2. \tag{13}$$

From this expression we can obtain the half life of any stimulation mode by evaluating the integral, and by setting $t = \tau_{1/2}$ when $n = n_0/2$. Specifically we now present new analytical expression for $\tau_{1/2}$ in three different types of stimulation: isothermal TL (ITL), continuous wave optically stimulated luminescence (CW-OSL) and linearly stimulated luminescence (LM-OSL).

3.1.1. Case of constant optical or thermal stimulation: $p(t) = \lambda$

In the case of isothermal TL decay (ITL) or CW-OSL processes, the excitation rate $p(t) = \lambda =$ constant. The parameter λ has of course a different meaning for each of these stimulation modes, representing thermal and optical processes correspondingly.

For these cases it is

$$\int_0^t p(t')dt' = \lambda t. \tag{14}$$

By setting $t = \tau_{1/2}$ when $n = n_o/2$ in Eq. (13) one obtains:

$$\tau_{1/2} = \frac{1}{\lambda}\left(\frac{NR}{n_0} + \ln 2(1-R)\right). \tag{15}$$

Eq. (15) gives the half life of the charge loss from a trap during an ITL or during a CW-OSL process. For $R = 0$ (case of no retrapping, and first order kinetics), this equation reduces to

$$\tau_{1/2} = \frac{\ln 2}{\lambda}, \tag{16}$$

i.e to the first order kinetics expression involving an exponential decay function, whereas for $R = 1$ it reduces to the second order kinetics expression:

$$\tau_{1/2} = \frac{1}{\lambda}\frac{N}{n_0}. \tag{17}$$

3.1.2. Case of linearly modulated stimulation: $p(t) = at$

In a Linearly Modulated OSL (LM-OSL) process the optical excitation probability is given by $p(t) = at$, where a is a constant with dimensions of s^{-1}, and which depends on the optical excitation probability and on the experimental setup. In this case:

$$\int_0^t p(t')dt' = \frac{at^2}{2}. \tag{18}$$

From Eqs. (13) and (18) one now obtains:

$$\tau_{1/2} = \sqrt{\frac{2}{a}\left(\frac{NR}{n_0} + \ln 2(1-R)\right)}. \tag{19}$$

Following the same mathematical procedure in the case of $R = A_n/A_m > 1$ (i.e. for the second branch of the Lambert function), it is found that the expressions for half lives are again Eqs. (15) and (19).

From the results of this section it becomes clear how one can obtain analytical expressions for $\tau_{1/2}$ in the OTOR model for *any* type of experimental stimulation mode.

3.2. An alternative derivation based on parametric equations of the OTOR model

An analytical expression for the half life $\tau_{1/2}$ within the OTOR model was obtained by Lovedy and Gartia (2013a), for the special case of isothermal stimulation with $\lambda =$ constant. In this section we follow the same method as these authors, but we do not assume that $\lambda =$ constant. It is also noted that the same method was used by Chen et al. (2010) in their dosimetry study of the OTOR model.

In this alternative method one starts from the following well-known GOT equation of the OTOR model, which is derived using the quasi-equilibrium (QE) conditions:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\frac{n^2\lambda}{RN + (1-R)n}. \tag{20}$$

By rearranging this equation:

$$\lambda\mathrm{d}t = -RN\frac{\mathrm{d}n}{n^2} - (1-R)\frac{\mathrm{d}n}{n}, \tag{21}$$

and integrating:

$$\int_0^t \lambda\mathrm{d}t = -RN\int_{n_o}^{n}\frac{\mathrm{d}n}{n^2} - (1-R)\int_{n_o}^{n}\frac{\mathrm{d}n}{n}, \tag{22}$$

$$\int_0^t \lambda \mathrm{d}t = RN\left(\frac{1}{n_o} - \frac{1}{n}\right) + (1-R)\ln\left(\frac{n_o}{n}\right). \tag{23}$$

This equation cannot be solved analytically for the concentration of trapped electrons $n(t)$ as a function of the elapsed time t, but it contains the relationship between n and t in parametric form.

By setting $t = \tau_{1/2}$ when $n = n_o/2$, one obtains:

$$\int_0^{\tau_{1/2}} \lambda \mathrm{d}t = \frac{RN}{n_o} + (1-R)\ln 2. \tag{24}$$

This equation is identical to the general Eq. (13) obtained in this paper by using the W function.

It is concluded that the two approaches (based on the W function and on the parametric equation for the OTOR) lead to the exact same analytical general Eq. (13), which can be used to find $\tau_{1/2}$ for any type of stimulation mode within the OTOR model.

It is noted that Lovedy and Gartia (2013a) followed the same method for the special case of isothermal stimulation with $\lambda =$ constant. Their Equation (16) reads:

$$t = \frac{1}{Q}\left(\frac{N\alpha}{(1-\alpha)n} - \frac{N\alpha}{(1-\alpha)n_o}\right) + \ln\left(\frac{n_o}{n}\right). \tag{25}$$

In their notation $\alpha = R$ and $Q = \lambda/(1-\alpha)$. By substituting this notation in the above equation, and by setting $t = \tau_{1/2}$ when $n = n_o/2$, we obtain:

$$\tau_{1/2} = \frac{1}{\lambda}\left(\frac{NR}{n_o}\right) + (1-R)\ln 2. \tag{26}$$

This is identical to Eq. (15), which was derived using the W function. However, it is noted that later in their paper Lovedy and Gartia (2013a) presented a different analytical equation for $\tau_{1/2}$ (their Eq. (20)), which we believe to contain an error, although their derivation method is correct.

3.3. Comparison of the analytical expressions for $\tau_{1/2}$ in the OTOR and GO models

It is useful to compare the OTOR expression for $\tau_{1/2}$ given by Eq. (15), with the previously derived general order kinetics expression for $\tau_{1/2}$. Furetta and Kitis (2004) started from the empirical general order equation:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -n^b\frac{s}{N^{b-1}}\exp(-E/kT), \tag{27}$$

and derived the following expression for $\tau_{1/2}$ during an ITL process:

$$\tau_{1/2} = \frac{1}{\lambda}\frac{N^{b-1}}{(1-b)n_0^{b-1}}\left(1 - \frac{1}{2^{1-b}}\right), \quad b \neq 1. \tag{28}$$

In the case of second order kinetics $b = 2$, Eq. (28) becomes

$$\tau_{1/2} = \frac{1}{\lambda}\frac{N}{(1-2)n_0}\left(1 - \frac{1}{2^{1-2}}\right), \tag{29}$$

which reduces to

$$\tau_{1/2} = \frac{1}{\lambda}\frac{N}{n_0}. \tag{30}$$

This is the same as Eq. (17), which was derived from the W function. This shows that the empirical general order kinetics approximates perfectly the behavior of the OTOR model in an ITL experiment, at the limits of $b \to 1$ and $b = 2$.

4. Analytical expressions for the temperature of maximum intensity T_m in a TL glow curve

As was discussed in the Introduction, the widely used Eq. (2) can not be solved analytically for the activation energy E, or for the temperature of maximum intensity T_m. In this section new analytical expressions are derived by using the W function, for the temperature T_m of maximum TL intensity (Section 4.1) and for the activation energy E (Section 4.2). The analytical equations are obtained in terms of the parameters in the OTOR model.

4.1. Analytical expression for T_m as a function of E, s, β, f_{gen}

Rearranging Eq. (2) we obtain

$$T_m^2 \exp\left(-\frac{E}{kT_m}\right) = \frac{\beta E}{kf_{gen}s}. \tag{31}$$

We take the logarithm of both sides:

$$2\ln(T_m) - \frac{E}{kT_m} = \ln\left(\frac{\beta E}{kf_{gen}s}\right), \tag{32}$$

$$\ln(T_m) - \frac{E}{2kT_m} = 0.5\ln\left(\frac{\beta E}{kf_{gen}s}\right), \tag{33}$$

$$-\ln\left(\frac{1}{T_m}\right) - \frac{E}{2kT_m} = 0.5\ln\left(\frac{\beta E}{kf_{gen}s}\right), \tag{34}$$

$$\ln\left(\frac{1}{T_m}\right) + \frac{E}{2kT_m} = -0.5\ln\left(\frac{\beta E}{kf_{gen}s}\right), \tag{35}$$

$$\ln\left(\frac{1}{T_m}\right) + \ln\left(\frac{E}{2k}\right) + \frac{E}{2kT_m} = \ln\left(\frac{E}{2k}\right) - 0.5\ln\left(\frac{\beta E}{kf_{gen}s}\right), \tag{36}$$

$$\ln\left(\frac{E}{2kT_m}\right) + \frac{E}{2kT_m} = \ln\left(\frac{E}{2k}\right) - 0.5\ln\left(\frac{\beta E}{kf_{gen}s}\right). \tag{37}$$

At this point we set

$$y_1 = \frac{E}{2kT_m}, \tag{38}$$

and

$$z_1 = \ln\left(\frac{E}{2k}\right) - 0.5\ln\left(\frac{\beta E}{kf_{gen}s}\right), \tag{39}$$

which can be further simplified after some algebra to:

$$z_1 = 0.5\ln\left(\frac{f_{gen}sE}{4k\beta}\right) = \ln\left(\sqrt{\frac{f_{gen}sE}{4k\beta}}\right), \tag{40}$$

Eq. (37) then takes the form

$$y_1 + \ln(y_1) = z_1, \tag{41}$$

which has the solution

$$y_1 = W_0[e^{z_1}]. \tag{42}$$

Taking into account the values of y_1 form Eq. (38) and of z_1 from Eq. (40), the final expression for evaluating T_m is obtained:

$$T_m = \frac{E}{2k}\frac{1}{W_0\left[\sqrt{\frac{f_{gen}sE}{4k\beta}}\right]}. \tag{43}$$

This is the desired analytical equation, which expresses T_m as a function of E, s, β, f_{gen}. The values of the parameter f_{gen} appearing in this equation are simulated and discussed in Section 5.1.

4.2. Analytical expressions for E as a function of T_m, s, β, f_{gen}

Eq. (2) can be also rearranged as follows:

$$\frac{E}{kT_m}\exp\left(\frac{E}{kT_m}\right) = \frac{f_{gen}sT_m}{\beta}. \tag{44}$$

Taking the logarithms of both sides:

$$\ln\left(\frac{E}{kT_m}\right) + \frac{E}{kT_m} = \ln\left(\frac{f_{gen}sT_m}{\beta}\right). \tag{45}$$

At this point we set

$$y_2 = \frac{E}{kT_m}, \tag{46}$$

and

$$z_2 = \ln\left(\frac{fsT_m}{\beta}\right), \tag{47}$$

Eq. (45) then takes the form

$$y_2 + \ln(y_2) = z_2, \tag{48}$$

which has the solution

$$y_2 = W_0[e^{z_2}]. \tag{49}$$

with z_2 given by Eq. (47).

Taking into account the value of y from Eq. (46) and of z_2 from Eq. (47), the final expression for E is:

$$E = kT_mW_0\left(\frac{f_{gen}sT_m}{\beta}\right). \tag{50}$$

This is the desired analytical equation, which expresses E as a function of T_m, s, β, f_{gen}. This equation is discussed further in Section 5.1.

4.3. Analytical expression for kinetic order b as a function of the integral symmetry factor μ'_g

According to Halperin and Branner (1960) and Kitis and Pagonis (2007) the integral symmetry factor μ'_g is defined as the ratio of the integral of the high temperature half of a TL peak, over the whole TL peak integral. Kitis et al. (2008) and Kitis and Pagonis (2007) obtained the following relationship between μ'_g and kinetics order b:

$$\mu'_g = \left[\frac{b}{1+(b-1)\frac{2kT_m}{E}}\right]^{-\frac{1}{b-1}} = \left[\frac{b}{f_{gen}}\right]^{-\frac{1}{b-1}}. \tag{51}$$

Taking the logarithm of both parts of Eq. (51) and after some algebra:

$$b\ln\left(\mu'_g\right) + \ln(b) = \ln\left(f_{gen}\mu'_g\right), \tag{52}$$

which can be written as

$$b\ln\left(\mu'_g\right) + \ln(b) + \ln\left(b\ln\left(\mu'_g\right)\right) - \ln\left(b\ln\left(\mu'_g\right)\right) = \ln\left(f_{gen}\mu'_g\right). \tag{53}$$

Eq. (53) is easily transformed to an equation of the form

$$y_3 + \ln(y_3) = z_3, \tag{54}$$

with

$$y_3 = b\ln\left(\mu'_g\right), \tag{55}$$

and

$$z_3 = \ln\left(f_{gen}\mu'_g\ln\left(\mu'_g\right)\right), \tag{56}$$

which has the solution

$$y = W_1[e^{z_3}], \tag{57}$$

where W_1 is the second real branch of the Lambert W function.

Taking into account Eqs. (55) and (56) we have

$$b = \frac{W_1\left[f_{gen}\mu'_g\ln\left(\mu'_g\right)\right]}{\ln\left(\mu'_g\right)}. \tag{58}$$

This is the desired analytical expression for the kinetic order b, as a function of the integral symmetry factor μ'_g. This equation also contains the parameter f_{gen} and is discussed in Section 5.

5. Results and discussion

All analytical expressions derived in the present work are summarized in Table 1.

The application of Eq. (15) to experimental results requires the values of R and n_0/N. It is noted that the value of R this can be obtained by curve fitting of experimental TL glow-curves using the OTOR TL expression by Kitis and Vlachos (2013) and by Sadek et al. (2015). The value of n_0 corresponds to the TL response at a dose D, and the value of N corresponds to the TL response when reaching a

Table 1
Summary of equation derived in this work using the Lambrt W function.

Quantity	Equation
General	$\int_0^{\tau_{1/2}} p(t')\mathrm{d}t' = \frac{NR}{n_0} + (1-R)\ln 2$
p(t) = λ	$\tau_{1/2} = \frac{1}{\lambda}\left(\frac{NR}{n_0} + \ln 2(1-R)\right)$
p(t) = a t	$\tau_{1/2} = \sqrt{\frac{2}{a}\left(\frac{NR}{n_0} + \ln 2(1-R)\right)}$
T_m	$T_m = \frac{E}{2k}W_0\left[\left(\frac{f_{gen}sE}{4k\beta}\right)^{\frac{1}{2}}\right]^{-1}$
E	$E = kT_mW_0\left[\frac{f_{gen}sT_m}{\beta}\right]$
b	$b = \frac{W_1[f_{gen}\mu'_g\ \ln(\mu'_g)]}{\ln(\mu'_g)}$
f_{gen}	$f_{gen} = a_0 + a_1\mu'^{a_2}_g$
f_{gen}	$a_0 = 0.965\pm0.006,\ a_1 = 0.677\pm0.09,\ a_2 = 3.147\pm0.02.$

saturation dose.

In the next two subsections we present simulations of the factor f_{gen} appearing in Eq. (2), and also test the validity of Eq. (58) for the kinetic order b by simulation.

5.1. Discussion of the factor f_{gen} appearing in Eq. (2)

In order to apply the analytical equations for the temperature T_m of maximum TL intensity (Section 4.1) and for the activation energy E (Section 4.2), one needs to consider the numerical factor f_{gen}.

Fig. 1 shows the coefficient f_{gen} as a function of the integral symmetry factor μ'_g. The values of f_{gen} were calculated by using 500 random values of possible $(E, s, n_o/N)$ triplets in the ranges shown in this figure.

The curve in Fig. 1 can be represented to a very accurate approximation by the equation:

$$f_{gen} = a_0 + a_1 \mu'^{a_2}_{g}, \tag{59}$$

where $a_0 = 0.965 \pm 0.006$, $a_1 = 0.677 \pm 0.09$ and $a_2 = 3.147 \pm 0.02$.

It is clear that f_{gen} varies by only 5% or less for a very wide range of possible values of the parameters in the model. In practice one could use as a good first approximation the value $f_{gen} = 1$. However the exact value of f_{gen} is very important for the correct evaluation of the kinetic order b (see next Section 5.2).

Sadek et al. (2015) showed that in the case of the OTOR model, the coefficient f_{gen} can be expressed by the following very good approximations

$$f_{Wm0} = \frac{1 - 1.05R^{1.26}}{1 - R}, \quad \textit{principal branch}, \tag{60}$$

$$f_{Wm1} = \frac{2.963 - 3.24R^{-0.74}}{|1 - R|}, \quad \textit{second branch}. \tag{61}$$

As it was shown by Kitis and Vlachos (2013), for the OTOR model $f_{gen} = f_{Wm0}$, so the expression for f_{Wm0} can also be used for general order kinetics without any loss of accuracy.

The analytical Eqs. (43) and (50) should be useful for researchers in this area of TL. Eq. (43) could be useful during theoretical work: when one has a chosen E, s pair, then one can find T_m easily from Eq. (43) by evaluating the argument of the Lambert W function and then evaluating the value of T_m by using any number of commercial software which contain the W function.

Similarly Eq. (50) should be useful in experimental or modeling work. For example, it is well known that at every experimental T_m value of a TL peak correspond theoretically an infinite number of (E, s) pairs. Since the value of T_m is known experimentally, and by assuming any value of the frequency factor s, one can use Eq. (50) to find the corresponding E. In curve fitting analysis of experimental TL curves, the initial guess values of (E, s) are very important. Therefore, Eq. (50) can help researchers find appropriate initial guess values for E, s.

5.2. Simulation of analytical expression for the kinetic order b

As was discussed previously in Section 5.1, the contribution of the value of the coefficient f_{gen} is minor when evaluating T_m and E using the new analytical equations. On the other hand, as will be shown below, the evaluation of b is extremely sensitive on the values of f_{gen}.

The validity of Eq. (58) was tested and verified extensively using many combinations of values $(E, s, n_0/N)$. A characteristic example is given in Fig. 2 for the case $n_o/N = 1$. The value of f_{gen} for a given b depends mainly on T_m. In the example of Fig. 2 the values of frequency factor was kept constant at $s = 10^{12}$ s^{-1}, whereas the values of activation energy E were 1, 1.25, 15, 1.75 and 2 eV. This combination of parameters simulates TL peaks having T_m values ranging from 400 K up to 800 K, so that it covers all the possible practical values of f_{gen}.

As it is seen in Fig. 2 there is excellent agreement between the b values from Eq. (51) represented by open circles, and the b values from Eq. (58) represented by the five indistinguishable solid lines corresponding to the five E-values used in the simulation. A similar results was also obtained by Gomez-Ros et al. (2006). The small disagreement appearing for $R < 0.06$ is a mathematical artifact of the simulation process, because during simulation it is not possible to obtain the integer value of $f_{gen} = 1$, but one obtains a slightly higher value. The consequence is that Eq. (50) will give b slightly above unity. However, the disagreement is not crucial, because in practical situations where $\mu'_g < 0.42$, one can set $b = 1$.

The great advantage of Eq. (58) is that it evaluates the kinetic order b using only the experimental value of the integral symmetry factor μ'_g. Traditionally researchers in the luminescence community have used the more familiar geometrical symmetry factor μ_g,

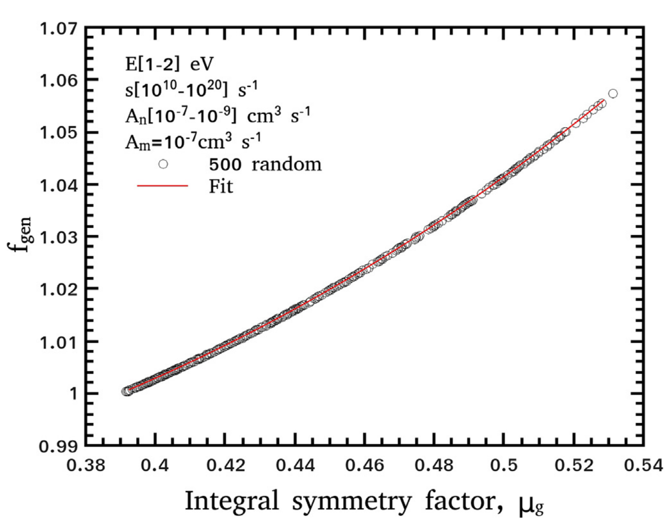

Fig. 1. The coefficient f_{gen} appearing in the evaluation of the condition for maximum intensity in a TL glow peak, as a function of the integral symmetry factor μ'_g.

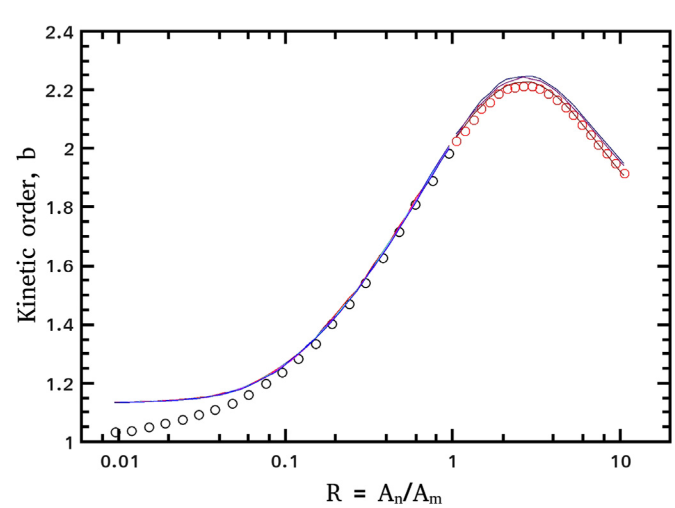

Fig. 2. Kinetic order b as a function of R. The open symbols correspond to b evaluated using Eq. (51), whereas the solid lines using Eq. (58).

instead of the integral symmetry factor μ'_g used in this equation (Chen and McKeever (1997)). It is also noted that for $b > 1$ the values of the two factors μ_g and μ'_g are very similar, as it was shown by Kitis et al. (2008).

6. Conclusions

The Lambert W function was used successfully by Kitis and Vlachos (2013) to obtain an analytical solution for the GOT equation of the OTOR model, and to obtain analytical expression for the intensity of a TL peak. In the present work the Lambert W function is used in four topics of the TL kinetics:

(a) To obtain an analytical expression for the half life of the charge loss in a single trap during an ITL, LM-OSL or CW-OSL process.
(b) To obtain an analytical expression for the temperature T_m of maximum TL intensity, as a function of the parameters E, s, β, f_{gen}.
(c) To obtain an analytical expression for the kinetic order b as a function of the experimentally obtained integral symmetry factor μ'_g.

The present work emphasizes the importance of the Lambert W function in TL kinetic theory. In our opinion, this function will have a major role in further developing the TL kinetic theory in the near future.

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