



# A new analytical equation for the dose response of dosimetric materials, based on the Lambert W function

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## ABSTRACT

The dose response of dosimetric materials is of fundamental importance in luminescence dosimetry and luminescence dating applications. In this paper we present a new analytical equation describing the trap filling process during irradiation of insulators, starting from the one trap and one recombination center model (OTOR). Even though this model has been studied extensively during the past 50 years, there are no published analytical solutions for the dose response  $n(D)$  in this model, where  $n$  is the concentration of filled traps and  $D$  is the irradiation dose. The new analytical equation contains the well-known Lambert function  $W$ , which has been used extensively during the past 20 years in diverse research areas. Under certain conditions, the new  $n(D)$  equation leads to the empirical saturating exponential function (SE). The new equation contains a smaller number of fitting parameters than two other commonly used fitting functions, the saturating exponential plus a linear function (SEL), and the double saturating exponential (DSE). In addition, the new equation contains physically meaningful parameters. Examples are shown of using the new equation to fit a variety of experimental signals, namely thermoluminescence (TL), optically simulated luminescence (OSL), isothermal TL (ITL) and electron spin resonance (ESR).

## 1. Introduction

The dose response of thermoluminescence (TL), isothermal thermoluminescence (ITL), optically stimulated luminescence (OSL) and electron spin resonance (ESR) signals is commonly shown as a graph of the intensity of these signals as a function of the irradiation dose. This type of graph is of fundamental importance in radiation dosimetry and luminescence dating. For a detailed bibliography on dose responses and the various published models, the reader is referred to the books by Chen and Pagonis [1], Chen and McKeever [2] and McKeever [3].

Experimentalists usually carry out two types of experiments, which measure two distinct types of dose responses. The first type of experiment measures the trapped charge *at the end of the irradiation process*, by using for example Electron Spin Resonance (ESR), or optical absorption techniques (OA). In this first type of experiment, the ESR and OA signals are usually assumed to be directly proportional to the concentration of filled traps  $n$  ( $\text{cm}^{-3}$ ) at the end of the irradiation process. In the second type of experiment, the trapped charge is measured at the end of two successive experimental stages, namely *at the end of irradiation followed*

*by thermal/optical stimulation* of the sample. Examples of this second type of experiment are measurements of dose response of TL, ITL and OSL signals. In these types of experiment, the stimulated luminescence signals may or may not be directly proportional to the concentration of filled traps at the end of the irradiation process, due to competition effects between traps and centers during the optical/thermal stimulation stage.

The simplest model describing the luminescence process during irradiation of a material is the one trap one recombination center model (OTOR). Although this model has been studied for more than 50 years, no *explicit analytical equation* exists to describe the dose response curves in the form  $n(D)$  within this model, where  $n$  ( $\text{cm}^{-3}$ ) is the concentration of filled traps and  $D$  (Gy) is the irradiation dose. The solution of the OTOR model for the irradiation process was given previously only as an *implicit parametric equation*  $D(n)$ , which must be inverted numerically to yield the dose response function  $n(D)$ . In the framework of the OTOR model, previous simulations have shown that  $n(D)$  has an initial linear dose response region for low doses, followed by a sublinear region in which the dose response varies as  $D^{1/2}$ , before approaching saturation

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(Lawless et al. [4]).

The goals of the present work are:

- To derive a new analytical expression for the dose response curves  $n(D)$  for the irradiation stage of the OTOR model, by using the well-known Lambert function  $W$  ([5,6]).
- To verify the new analytical equation, by comparing it with the numerical solution of the differential equations in the OTOR model.
- To compare the new equation with three commonly used data fitting functions: the saturating exponential (SE), saturating plus linear (SEL) and double saturating exponential (DSE) fitting equations.
- To fit previously published experimental data for TL, OSL, ESR and ITL signals with the new analytical equation.

This paper is organized as follows. Section 2 derives and verifies the new analytical equation for the dose response  $n(D)/N$ , within the framework of the OTOR model. Section 3 explores the relationship between the new Lambert solution and the saturating exponential function. Section 4 presents fits of previously published experimental data by using the new analytical equation. The paper concludes with a general discussion of the new dose response equation, and of the importance of the Lambert function in describing luminescence phenomena.

## 2. Derivation of the new analytical dose response equation

Fig. 1 shows a schematic diagram of the OTOR model, and the relevant electronic transitions during the irradiation of a sample. The differential equations governing the traffic of electrons between the trapping level, the recombination center and the conduction band in the OTOR model are [1]:

$$\frac{dn}{dt} = A_n(N - n)n_c, \quad (1)$$

$$\frac{dm}{dt} = B(M - m)n_v - A_m m n_c, \quad (2)$$

$$\frac{dn_c}{dt} = X - A_n(N - n)n_c - A_m m n_c, \quad (3)$$

$$\frac{dn_v}{dt} = \frac{dn}{dt} + \frac{dn_c}{dt} - \frac{dm}{dt}. \quad (4)$$

$$m + n_v = n + n_c. \quad (5)$$

Here  $n$  ( $\text{cm}^{-3}$ ) and  $m$  ( $\text{cm}^{-3}$ ) are the concentrations of electrons in

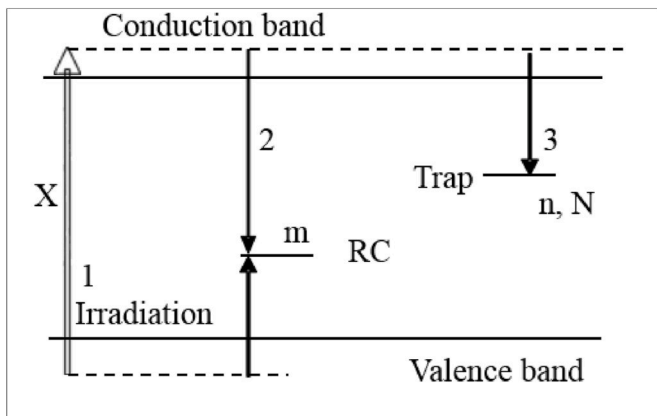


Fig. 1. The OTOR model showing the various electronic transitions during the irradiation process. Transition (1): Creation of electron-hole pairs by radiation. Transition (2): Trapping of holes and recombination of electrons at the recombination centers (RC), Transition (3): Trapping of electrons in the dosimetric trap.

traps and of holes in recombination centers respectively, and  $N$  and  $M$  ( $\text{cm}^{-3}$ ) are the total concentrations of trapping states and recombination centers.  $n_c$  ( $\text{cm}^{-3}$ ) and  $n_v$  ( $\text{cm}^{-3}$ ) are respectively the concentrations of free electrons and holes.  $A_n$  ( $\text{cm}^3\text{s}^{-1}$ ) is the retrapping coefficient of electrons,  $A_m$  ( $\text{cm}^3\text{s}^{-1}$ ) the recombination coefficient of electrons, and  $B$  ( $\text{cm}^3\text{s}^{-1}$ ) the trapping coefficient of holes in centers.  $X$  ( $\text{cm}^{-3}\text{s}^{-1}$ ) is proportional to the dose-rate of excitation, and actually denotes the rate of production of electron-hole pairs by the excitation irradiation per unit volume per second. Eq. (5) is the charge neutrality condition.

The above set of equations cannot be solved analytically. Instead, one uses the quasi-equilibrium (QE) assumption, to transform them into a single differential equation, as follows. The QE assumption requires that the free electron and free hole concentrations in the conduction and valence bands are quasi-stationary, and is mathematically expressed as ([1]):

$$\left| \frac{dn_c}{dt} \right| \ll \left| \frac{dn}{dt} \right|, \quad \left| \frac{dn_v}{dt} \right| \ll \left| \frac{dm}{dt} \right| \quad \text{and} \quad n_c \ll n, \quad n_v \ll m. \quad (6)$$

In practice, this means that the concentration of  $n_c$  in the conduction band and the concentration  $n_v$  in the valence band are almost constant in time, and this allow us to set:

$$\frac{dn_c}{dt} \simeq \frac{dn_v}{dt} \simeq 0. \quad (7)$$

By setting  $dn_c/dt = 0$  in Eq. (3), the  $n_c$  values under the QE conditions are:

$$n_c = \frac{X}{A_n(N - n) + m A_m}. \quad (8)$$

By replacing  $n_c$  from Eq. (8) into Eq. (1) and since  $n \simeq m$ , the following single differential equation is obtained:

$$\frac{dn}{dt} = \frac{(N - n)A_n}{(N - n)A_n + n A_m} X. \quad (9)$$

This equation was derived and integrated previously for example by Lawless et al. [4], who showed that it can be easily integrated by separation of variables, to yield (Ref. [4], their Eq. (11)):

$$Xt = n + \frac{A_m}{A_n} \left[ -N \ln \left( 1 - \frac{n}{N} \right) - n \right]. \quad (10)$$

The product  $D = Xt$  represents the irradiation dose received by the sample, and by introducing the dimensionless retrapping ratio  $R = A_n/A_m$  in this equation, we obtain:

$$D = n + \frac{1}{R} \left[ -N \ln \left( 1 - \frac{n}{N} \right) - n \right]. \quad (11)$$

This is an equation for  $D(n)$ , which has been inverted numerically by previous researchers, in order to plot the inverse function  $n(D)$ . Lawless et al. [4] developed *approximate* solutions of this equation for low doses and high doses. We now develop the *exact* analytical solution  $n(D)$  of this equation in terms of the Lambert  $W$  function, as follows. We rewrite Eq. (11) as:

$$\frac{RD}{N} = \frac{n}{N} (R - 1) - \ln \left( 1 - \frac{n}{N} \right), \quad (12)$$

and introduce the trap filling ratio  $x = n/N$  to obtain:

$$\ln(1 - x) + (1 - R)x = -\frac{RD}{N}. \quad (13)$$

We note that this equation is of the general algebraic form:

$$\ln(a + bx) + cx = \ln d, \quad (14)$$

which has the analytical solution (see for example the websites dedicated to the Lambert function [7,8]):

$$x = \frac{1}{c} W \left[ \frac{cd}{b} \exp \left( \frac{ac}{b} \right) \right] - \frac{a}{b}. \quad (15)$$

The term inside the square brackets in this equation is the argument of the Lambert function  $W[z]$ . By substituting  $a = 1$ ,  $b = -1$ ,  $c = 1 - R$ ,  $\ln d = -RD/N$  (or  $d = \exp(-RD/N)$ ), we obtain:

$$\frac{n(D)}{N} = 1 + \frac{W[(R-1)\exp(R-1-RD/N)]}{1-R}. \quad (16)$$

By defining a constant  $D_c$  such that:

$$D_c = N/R, \quad (17)$$

Eq. (16) becomes:

$$\frac{n(D)}{N} = 1 + \frac{W[(R-1)\exp(R-1-D/D_c)]}{1-R}. \quad (18)$$

This is the desired new analytical expression for the irradiation stage of the OTOR model, which gives the trap filling ratio  $n(D)/N$  as a function of the dose  $D$ , by using the Lambert function. It shows that the function  $n(D)/N$  depends only on two parameters, i.e. on the retrapping ratio  $R$  and on the constant  $D_c = N/R$ . The parameter  $D_c$  has the same units as the dose  $D$ , and depends on the physical properties  $R, N$  of the material.

The values  $R \ll 1$  and  $R = 1$  correspond to first and second order kinetics. Furthermore, under certain physical assumptions, values of  $R$  between 0 and 1 correspond to the empirical general order intermediate kinetic orders (see for example the discussion in Kitis et al. [9]). However, it is noted that from a physical point of view, the retrapping ratio parameter  $R$  can have any positive real value, including values  $R > 1$ .

Fig. 2 shows plots of  $n(D)/N$  from Eq. (18) as a function of the normalized dose  $D/D_c$ , for values of the retrapping ratio between  $R = 10^{-2}$  and  $R = 10$  (solid lines). The open symbols in this figure represent the numerical solution of the differential Eq. (9), showing excellent agreement between the numerical solution and the new analytical Eq. (18). As may be expected from a physical point of view, the approach to saturation and the shape of the  $n(D)$  function depends on the amount of retrapping, i.e. on the value of the ratio  $R$ .

We can check the behavior of the analytical solution at  $D = 0$ , by noting that  $n(0)/N = 1 + W[(R-1)\exp(R-1)/(1-R)]$ . Since  $W(u \exp u) = u$  for any value of  $u$ , then  $W[(R-1)\exp(R-1)] = R-1$  and we obtain  $n(0)/N = 1 + (R-1)/(1-R) = 0$ . This is consistent with the initial condition of empty traps  $n(0) = 0$ .

If the traps are not initially empty (i.e.  $n(0) = n_0 \neq 0$ ), the solution of Eq. (18) is found using the same method to be:

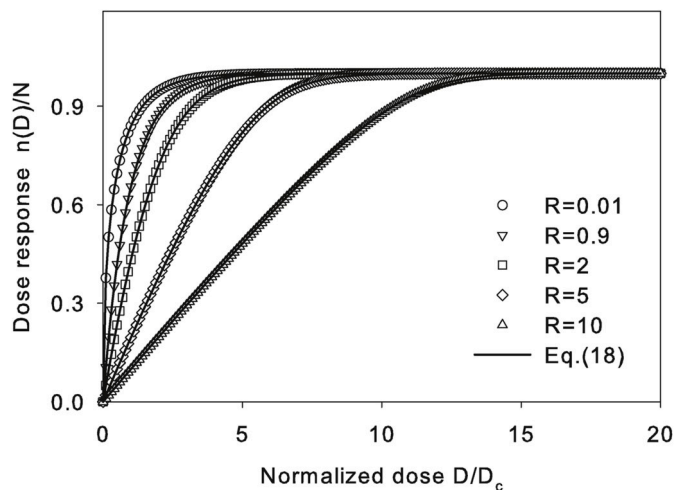


Fig. 2. Plots of the analytical Eq. (18) (solid lines) for several values of the retrapping ratio  $R$ , as a function of the normalized dose  $D/D_c$ . The open symbols are the numerical solution of the differential Eq. (9).

$$\frac{n(D)}{N} = 1 + \frac{W[(R-1)(1-n_0/N)\exp(R-1+n_0/N-D/D_c)]}{1-R}. \quad (19)$$

By setting  $n_0 = 0$  in Eq. (19) one obtains Eq. (18), as expected. By collecting terms, the previous equation can be written as:

$$\frac{n(D)}{N} = 1 + \frac{W[(R-1)\exp(R-1+n_0/N+\ln(1-n_0/N)-D/D_c)]}{1-R}, \quad (20)$$

or

$$\frac{n(D)}{N} = 1 + \frac{W[(R-1)\exp(R-1-(D+D_{int})/D_c)]}{1-R}, \quad (21)$$

where the constant  $D_{int}$  has the same dimensions as the irradiation dose  $D$ , and is defined by:

$$D_{int} = D_c[n_0/N + \ln(1-n_0/N)]. \quad (22)$$

Equation (21) has the exact same mathematical form as Eq. (18), but is shifted along the horizontal  $D$ -axis by the amount  $D_{int}$  given by Eq. (22).

In Section 4, Eq. (18) will be used to fit experimental data which start at the origin, while Eq. (21) will be used to fit experimental data which have a non-zero intercept on the  $y$ -axis.

An important question is whether the QE conditions still apply for the large values of  $R > 1$  used in the simulations of Fig. 2. The applicability of QE conditions was tested by comparing the numerical solution of the kinetic rate equations (1)–(4), with the analytical Lambert solution Eq. (18). This was done for a range of  $R$  values between  $R = 0.001$  and  $R = 10$ , and the agreement of the two solutions was better than 1% for the complete dose response curve shown in Fig. 2. This agreement confirms that Eq. (18) is indeed consistent with the QE conditions, and can be applied for all values of  $R$ .

### 3. The relationship between the Lambert $W$ and the saturating exponential function

The shape of the simulated dose response  $n(D)/N$  shown in Fig. 2 depends strongly on the retrapping ratio  $R$ , and looks similar to a saturating exponential function (SE). The SE is often used to fit experimental dose responses in a variety of materials, and for a variety of luminescence signals. Its general form is ([10–12]):

$$\frac{n(D)}{N} = 1 - \exp \left[ -\frac{D}{D_o} \right], \quad (23)$$

where  $D_o$  is called the characteristic dose of the trap filling process.

For many dosimetric materials, it is found that the dose response cannot be described by a SE, and researchers frequently use two more general equations, the SEL and DSE functions written as (Berger and Chen [13]):

$$\frac{n(D)}{N} = B_1 D + B_2 \left( 1 - \exp \left[ -\frac{D}{D_o} \right] \right), \quad (24)$$

$$\frac{n(D)}{N} = B_3 \left( 1 - \exp \left[ -\frac{D}{D_{o2}} \right] \right) + B_4 \left( 1 - \exp \left[ -\frac{D}{D_{o1}} \right] \right), \quad (25)$$

where  $B_i$  ( $i = 1 \dots 4$ ) are constants, and  $D_{oi}$  are two constants characteristic of the sample with the dimensions of dose, respectively. It is important to note that the SE, SEL and DSE are considered more or less empirical analytical equations, and the constants  $B_i$  are not usually assigned a direct physical meaning. We now explore the relationship between the SE and the analytical solution in Eq. (18).

The argument of the Lambert function in Eq. (18) is the parameter  $z = (R-1)\exp[R-1-D/D_c]$ , which is a function of the dose  $D$ . In cases where this parameter  $|z| \ll 1$ , one can use the series approximation  $W(z) \cong z$  for the Lambert function in Eq. (18), to obtain:

$$\frac{n(D)}{N} \cong 1 + z \left/ (1 - R) = 1 + (R - 1)\exp(R - 1 - D/D_c) \right/ (1 - R), \quad (26)$$

$$\frac{n(D)}{N} \cong 1 - \exp(R - 1 - D/D_c). \quad (27)$$

This equation has the same mathematical form as the saturating exponential in Eq. (23), except for the extra term  $\exp(R - 1)$  multiplying the exponential term  $\exp(-D/D_c)$ . When  $\exp(R - 1) \cong 1$ , i.e. when  $R \cong 1$ , the Lambert dose response equation in Eq. (18) becomes identical with the SE in Eq. (23), and the two respective dose constants become equal ( $D_o = D_c$ ). However, for small or large values of  $R$ , (e.g. when  $R = 0.001$  or  $R = 3$ ), this extra  $\exp(R - 1)$  factor will produce a disagreement between the two expressions.

Fig. 3 shows plots of dose response curves  $n(D)/N$  by using Eq. (18), for  $R = 0.01, 0.5, 0.1, 2$ . These  $n(D)/N$  curves are fitted here with the SE function in Eq. (23), for comparison purposes. It is clear from this figure that significant differences between the SE and the new dose response equation appear for small or large values of  $R$ , while the two functions agree very closely for values of  $R \cong 1$ . This indicates that the new dose response equation based on the Lambert function is a more general flexible equation, which can be used to describe a variety of shapes of dose response data.

In the next section we will use the Lambert dose response function Eq. (18) and Eq. (21), in order to fit published experimental data for a variety of luminescence signals in various dosimetric materials.

#### 4. Fitting experimental data with the new Lambert dose response function Eq. (18) and Eq. (21)

The experimental data presented in this section were chosen as representative cases in the bibliography, which could not be fitted with a SE function, and required instead the use of a SEL or a DSE fitting function. As will be shown here, the new analytical Eq. (18) provides a satisfactory alternative to the empirical SEL and DSE regression models used previously in the literature. The experimental data shown in Figs. 4–7 were reproduced for the purposes of this paper from the original papers, by using digitizing software.

Berger and Chen [13] considered OSL signals, which were measured using the single-aliquot regenerative dose protocol (SAR) on fine grain sedimentary quartz. They showed that their signals could not be fitted using SE functions, but one should use instead the SEL Eq. (24), or the

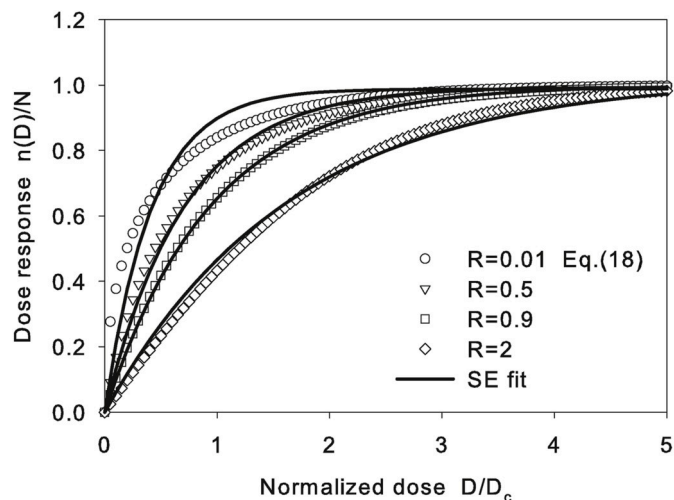


Fig. 3. Plots of the new Lambert dose response function in Eq. (18) shown as open symbols, and of the corresponding least squares fits using the empirical SE function (27) shown as solid lines. Significant differences are seen between Eq. (18) and the SE function, with agreement between the two functions occurring only for values  $R \cong 1$ .

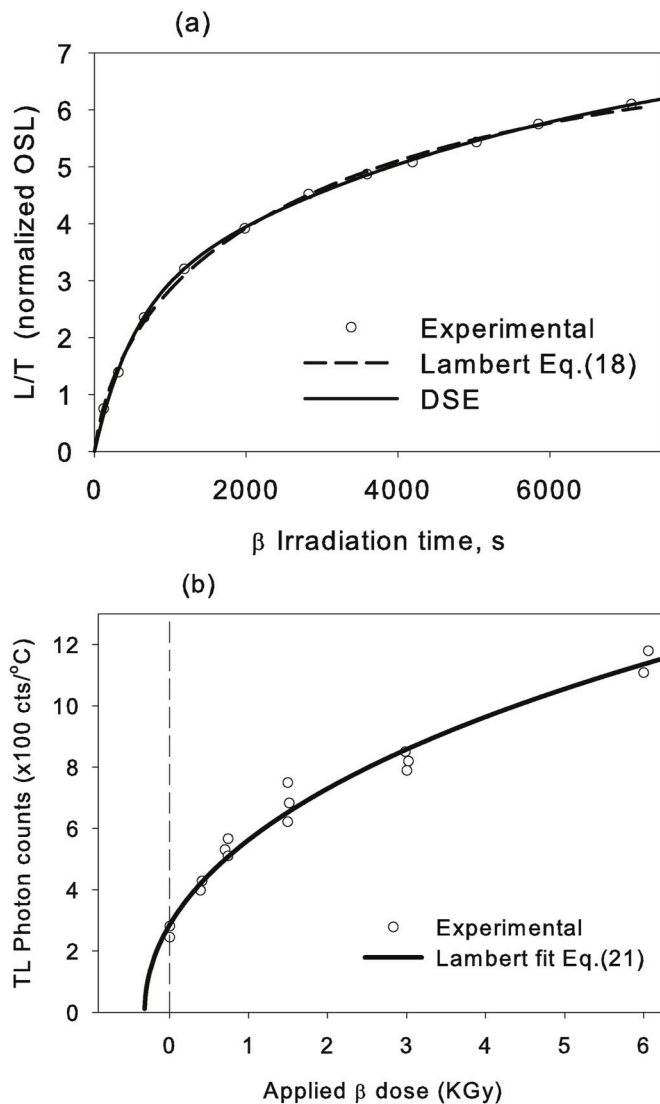


Fig. 4. (a) Fit to the normalized OSL SAR data by Berger and Chen [13], using Eq. (18). This set of OSL data starts at the origin. (b) Fit to the TL data by Berger [14], by using the new dose response Eq. (21), and also by using a DSE. This set of additive-dose TL data has a non-zero y-intercept, corresponding to the equivalent dose  $D_E$ .

DSE Eq. (25). These authors showed clearly that the DSE regression model fitted the OSL dose response data better than by the other two models. In addition to the comparison with experiment, Berger and Chen [13] also showed that a simulated dose response from the OTOR model also could not be fitted accurately using the SE and SEL functions, and required the use of a DSE.

Fig. 4a shows the OSL data from Berger and Chen [13], their Fig. 1. A preheat of 240 °C was employed during the SAR protocol, and the beta dose rate was 0.12 Gy/s. The two lines fitted to the data are the Lambert Eq. (18), and the DSE function used by Berger and Chen [13]. The two lines are indistinguishable, however it is important to note that the Lambert fitting function contains only two parameters ( $R, D_c$ ), while the DSE Eq. (25) requires 4 fitting parameters.

Fig. 4b shows a set of TL data from Berger [14], their Fig. 1. This is a set of additive-dose data for purified volcanic glass, measured at the 321–330 °C temperature range of the glow curves, and preheated for 8 days to remove unstable TL. This type of additive-dose data often contains a non-zero y-intercept, therefore the fitting procedure introduces an extra fitting parameter. The data in this figure was fitted with the Lambert Eq. (21), with the x-intercept represents the equivalent dose  $D_E$

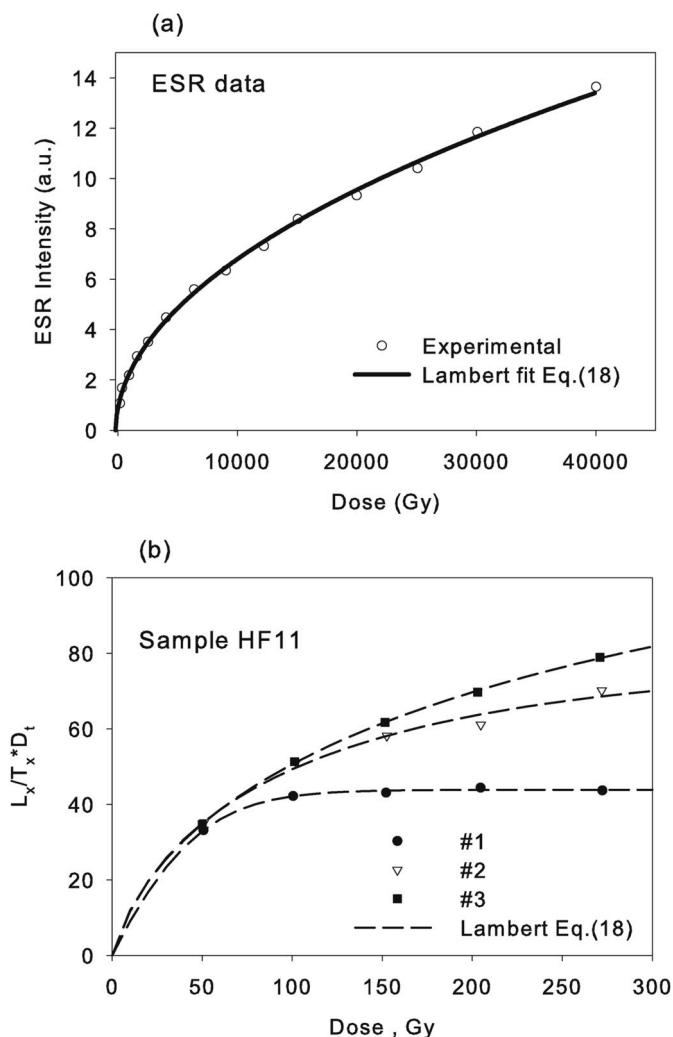


Fig. 5. (a) Fit to ESR data from Duval [15], by using the new dose response Eq. (18). (b) Test dose-corrected OSL signals from sample HF11 in Li et al. [22]. The solid lines indicate the least squares fits using the new Eq. (18).

for this sample.

In more recent experimental work, the SEL and DSE functions have been used to fit experimental ESR data (Duval [15], Trompier et al. [16]), OSL data (Lowick [17], Timar-Gabor et al. [18,19], Anechitei-Deacu et al. [20], Fuchs [21], Li et al. [22]), TL data (Berger and Chen [13], Berger [14], Bösken and Schmidt [23]), and ITL data (Vandenberghe et al. [24]).

Fig. 5a shows ESR experimental data from Duval [15], by using the new dose response Eq. (18). These authors measured the dose response curves (DRCs) of the Al center from 15 sedimentary quartz samples from the Iberian Peninsula. The samples were irradiated in 11–14 dose steps up to a maximum dose of 23–40 kGy. It was found that the ESR signal grows almost linearly with the absorbed dose for doses above ~4 kGy. In this study it was concluded that the ESR signal contains at least two components, with the first component saturating at low doses and the second component showing no saturation even at these very high doses. The solid line in Fig. 5a is the least squares fits using the new Eq. (18). The observed good fit to the experimental data suggests that the ESR signal may contain a single component, which can be described by the new dose response function based on the Lambert function.

Fig. 5b shows typical test dose-corrected OSL signals from three aliquots of sample HF11 studied by Li et al. [22]. These authors fitted the data set for aliquots #1 and #2 using a single SE function, while the data for aliquot #3 was fitted using a single SEL function plus an extra linear

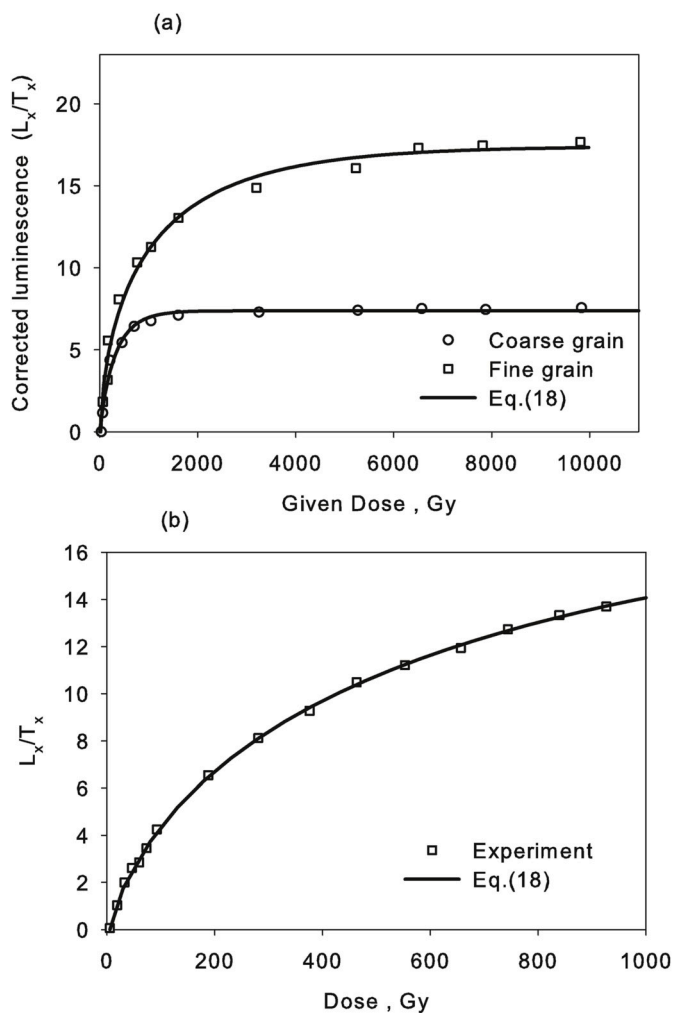


Fig. 6. Fit to OSL SAR data by (a) Timar-Gabor et al. [18] and (b) Lowick [17].

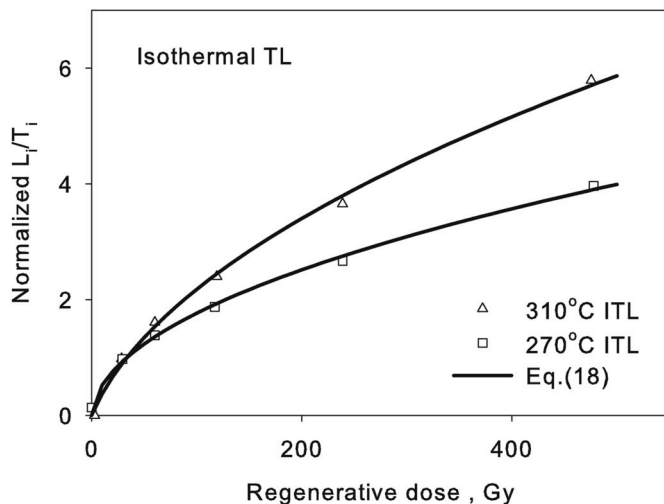


Fig. 7. Fit to isothermal TL SAR data from Vandenberghe et al. [24].

term. The solid lines indicate the least squares fits using the new Eq. (18). The good fit to the different experimental behaviors in this figure shows the flexibility of the Lambert dose response function, which can be used to fit the variety of OSL dose response behaviors seen in a typical quartz single grain SAR protocol.

Fig. 6a shows SAR-OSL experimental dose response curves by Timar-Gabor et al. [18] (their Fig. 3), for fine grain and coarse grain quartz samples in a loess-palaeosol sequence. The data shown here for samples MV 10 and MV 8, and were fitted by the authors using a DSE. The solid lines in Fig. 6a are the least squares fits using the new Eq. (18), showing that the Lambert function can be used to describe both types of dose responses in quartz with a smaller number of parameters than the DSE, even at the high doses involved in this experiment.

Similar data by Lowick [17] are shown in Fig. 6b, for a fine grained quartz sample NWG11, measured using a modified SAR protocol with a test dose of 18.6 Gy. Lowick [17] fitted this data using a SEL function; the solid line is the least squares fit using the new Eq. (18).

Fig. 7 shows ITL experimental data by Vandenberghe et al. [24], fitted using the Lambert Eq. (18). ITL measurements were performed by holding the aliquots for 600 s at a fixed temperature, after they had been preheated for 10 s at 300 °C. The ITL curves were recorded as soon as the measurement temperature was reached. Once more, the experimental data for this different type of experiment can be fitted accurately using the new Lambert dose response function.

The analytical Eq. (18) derived in this paper describes the dose response of the population of trapped electrons  $n(D)$  at the end of the irradiation stage. One would then expect that this equation can be used to describe the dose response of ESR data, which are assumed to be proportional to the dose response  $n(D)$ . In this section it was shown that Eq. (18) can also be used to describe the dose response of the luminescence signal  $I(D)$  measured during a TL, ITL or OSL experiment. The luminescence intensity in the OTOR model is proportional to  $n$  only for first-order kinetics, and therefore one would expect fitting of the experimental data to yield values of  $R < 1$ . The values of  $R$  and  $D_c$  for the fits in Figs. 5–7 are summarized in Table 1. The data in this Table show that the condition  $R < 1$  is indeed satisfied in all cases, except in one case for which the value of  $R = 1.86$  was obtained. This shows that using Eq. (18) to fit luminescence intensity is consistent with the assumption of first order kinetics.

## 5. Discussion

The existing models of nonlinear dose response  $n(D)$  in dosimetric materials are usually classified into two major categories. Models in the first category describe the dose response  $n(D)$ , on the basis of mechanisms taking place during the irradiation stage. Such models provide an explanation for, among others, nonlinearity effects of ESR and OA measurements. Models in the second category describe nonlinearity effects as a result of competition mechanisms occurring during the readout stage, i.e. during the optical or thermal stimulation of the previously irradiated sample.

The analytical equation in this paper belongs to the first group of models, and can not provide an explanation for superlinearity effects, since there are no competing traps included in the OTOR model. Analytical expressions for  $n(D)$  from models based on the irradiation stage, were previously proposed by Waligórski et al. [25,26], based on the track structure theory of Katz [27]. These previously used dose response curves have the form of a saturating exponential.

Levy [28] presented a phenomenological explanation of the origin of the SEL and DSE dose response functions, and how they can be used to describe the trap filling process. The proposed physical mechanism by Levy [28] is the creation of additional traps during the irradiation of the samples.

## 6. Summary and conclusions

In this paper, a new analytical equation describing the trap filling ratio  $n(D)/N$  was derived within the OTOR model, by using the Lambert function. The Lambert function was used by Kitis and Vlachos [29] to solve the OTOR model during the readout stage, in order to obtain an analytical expression for TL, OSL etc. Later Lovedy et al. [30,31] also

**Table 1**

Summary of the best fitting values  $R$ ,  $D_c$  from using Eq. (18) to fit the experimental data in Figs. 4–7.

Figure in this paper	Type of data	$R$	$D_c$ (Gy)	Reference
4a	OSL (SAR)	0.114	6467.7	[13]
4b	TL	$0.42 \times 10^{-8}$	$68.8 \times 10^3$	[14]
5a	ESR	0.00043	$1.43 \times 10^7$	[15]
5b (curve #1)	OSL	1.86	24.6	[22]
5b (curve #2)		0.28	182.7	[22]
5b (curve #3)		0.12	598.8	[22]
6a (Coarse grain)	OSL	0.721	379.7	[18]
6a (Fine grain)	OSL	0.133	2166.5	[18]
6b	OSL	0.208	1245.4	[17]
7 (curve 310 °C)	ITL	0.0088	$3.42 \times 10^5$	[24]
7 (curve 270 °C)	ITL	0.00085	$3.85 \times 10^5$	[24]

solved the OTOR model using the equivalent Wright  $\omega$  function. In all modern software these functions are built-in functions like the common transcendental functions of sine, cosine, logarithm etc. Recently the applications of the  $W$  function in phenomenological luminescence models (TL, OSL etc) were reviewed by Kitis et al. [9]. For a general discussion of the properties of the  $W$  function and its many uses in science, the reader is referred to the original papers by Corless ([5,6]).

The new analytical Eq. (18) was verified by comparing with the numerical solution of the corresponding differential equation, and is characterized by the retrapping ratio  $R$  in the model. For values of  $R \cong 1$  the new analytical equation can be approximated very well by a SE function, while for  $R \leq 0.1$  or  $R > 1$  the two functions diverge significantly.

The results of the previous sections showed that the new dose response function in Eqs. (18) and (21) are more general functions than the SE, SEL and DSE equations. In addition, the proposed fitting function contains a smaller number of parameters than the SEL and DSE, and is based on the physically meaningful parameters  $R$ ,  $D_c$  instead of empirical constants.

From a physical point of view, the new equation provides a simpler interpretation of the shape of the dose response curve, than the SEL and DSE. This is because it is not necessary to invoke the presence of *two components/traps* during the irradiation and the luminescence process, as is common practice when using the SEL and DSE. In the new interpretation provided by Eq. (18), the experimental data represent the dose response of a *single trap*, instead of the two traps implied in the DSE and SEL functions.

The new analytical equation can stand alone, in the sense that it can be used to describe different dose behaviors, independently of the OTOR model. However, it can *not* be used to fit superlinearity phenomena, since these are due to competition effects which are not included in the OTOR model.

## Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## CRediT authorship contribution statement

**Vasilis Pagonis:** Conceptualization, Methodology, Software, Writing - review & editing. **George Kitis:** Conceptualization, Methodology, Software, Writing - review & editing. **Reuven Chen:** Conceptualization, Methodology, Software, Writing - review & editing.

## References

- [1] R. Chen, V. Pagonis, *Thermally and Optically Stimulated Luminescence: A Simulation Approach*, Wiley and Sons, Chichester, 2011.

- [2] R. Chen, S.W.S. McKeever, *Theory of Thermoluminescence and Related Phenomena*, World Scientific, 1997.
- [3] S.W.S. McKeever, *Thermoluminescence of Solids*, Cambridge University Press, Cambridge, 1985.
- [4] J.L. Lawless, R. Chen, V. Pagonis, Sublinear dose dependence of thermoluminescence and optically stimulated luminescence prior to the approach to saturation level *Radiat. Meas.* 44 (2009) 606–610.
- [5] R.M. Corless, G.H. Gonnet, D.G.E. Hare, D.J. Jeffrey, D.E. Knuth, On the Lambert W function, *Adv. Comput. Math.* 5 (1996) 329–359.
- [6] S.R. Valluri, D.J. Jeffrey, R.M. Corless, Some applications of the Lambert W function in physics, *Can. J. Phys.* 78 (2000) 823–831.
- [7] E.W. Weisstein, Lambert W-function.” from MathWorld—A wolfram web resource, 3/3/2020, <http://mathworld.wolfram.com/LambertW-Function.html>.
- [8] K. Briggs, W-ology, or, some exactly solvable growth models, 3/3/2020, <http://keithbriggs.info/W-ology.html>.
- [9] G. Kitis, G. S Polymeris, V. Pagonis, Stimulated luminescence emission: from phenomenological model to master analytical equations, *Appl. Radiat. Isot.* 153 (2019) 108797.
- [10] R. Grün, P.D.M. Macdonald, Non-linear fitting of TL/ESR dose-response curves, *International Int. J. Radiat. Appl. Instrum. A. Applied Radiation and Isotopes* 40 (1989) 1077–1080.
- [11] R. Grün, Dose response of the paramagnetic centre at  $g = 2.0007$  in corals, *Ancient TL* 8 (3) (1990) 20–22.
- [12] P. Guibert, E. Vartanian, F. Bechtel, M. Schvoerer, Non linear approach of TL response to dose: polynomial approximation, *Ancient TL* 14 (2) (1996) 7–14.
- [13] G.W. Berger, R. Chen, Error analysis and modelling of double saturating exponential dose response curves from SAR OSL dating, *Ancient TL* 29 (2) (2011) 9–14.
- [14] G.W. Berger, Regression and error analysis for a saturating-exponential-plus-linear model, *Ancient TL* 8 (3) (1990) 23–25.
- [15] M. Duval, Dose response curve of the ESR signal of the Aluminum center in quartz grains extracted from sediment, *Ancient TL* 30 (2) (2012) 1–9.
- [16] F. Trompieri, C. Bassinet, A. Wieser, C. De Angelis, D. Viscomi, P. Fattibene, Radiation-induced signals analysed by EPR spectrometry applied to fortuitous dosimetry, *Ann. Ist. Super Sanita* 45 (2009) 287–296.
- [17] S.E. Lowick, F. Preusser, A.G. Wintle, Investigating quartz optically stimulated luminescence dose–response curves at high doses, *Radiat. Meas.* 45 (2010) 975–984.
- [18] A. Timar-Gabor, Ş. Vasiliniuc, D.A.G. Vandenberghe, C. Cosma, A.G. Wintle, Investigations into the reliability of SAR-OSL equivalent doses obtained for quartz samples displaying dose response curves with more than one component, *Radiat. Meas.* 47 (2012) 740–745.
- [19] A. Timar-Gabor, D. Constantin, J.P. Buylaert, M. Jain, A.S. Murray, A.G. Wintle, Fundamental investigations of natural and laboratory generated SAR dose response curves for quartz OSL in the high dose range, *Radiat. Meas.* 81 (2015) 150–156.
- [20] Anechitei-Deacu, A. Timar-Gabor, K.J. Thomsen, J.P. Buylaert, M. Jain, M. Bailey, A.S. Murray, Single and multi-grain OSL investigations in the high dose range using coarse quartz, *Radiat. Meas.* 120 (2018) 124–130.
- [21] M. Fuchs, S. Kreutzer, D. Rousseau, P. Antoine, C. Hatté, O. Moine, C. Gauthier, J. Svoboda, L. Lisá, Left the loess sequence of Dolní Věstonice, Czech Republic: a new OSL-based chronology of the Last Climatic Cycle, right Boreas 42 (2013) 664–677.
- [22] B. Li, Z. Jacobs, R.G. Roberts, Investigation of the applicability of standardised growth curves for OSL dating of quartz from Haua Fteah cave, Libya, *Quat. Geochronol.* 35 (2016) 1–15.
- [23] J.J. Bösken, C. Schmidt, Direct and indirect luminescence dating of tephra: a review, *J. Quat. Sci.* (2019) 1–15.
- [24] D.A.G. Vandenberghe, M. Jain, A.S. Murray, Equivalent dose determination using a quartz isothermal TL signal, *Radiat. Meas.* 44 (2009) 439–444.
- [25] M.P.R. Waligórski, R. Katz, Supralinearity of peak 5 and peak 6 in TLD-700 Nucl, *Instrum. and Methods* 172 (1980) 463–470.
- [26] M.P.R. Waligórski P. Olko, P. Bilski, M. Budzanowski T, Niewiadomski Dosimetric characteristic of LiF:Mg,Cu,P phosphors - a track structure interpretation, *Radiat. Protect. Dosim.* 47 (1993) 53–58.
- [27] R. Katz, Track structure theory in radiobiology and radiation protection Nucl, *Track Det* 2 (1978) 1–28.
- [28] P.W. Levy, Overview of nuclear radiation damage processes: phenomenological features of radiation damage in crystals and glasses, in: Paul W. Levy (Ed.), *Radiation Effects on Optical Materials*, SPIE, 1985, pp. 2–24.
- [29] G. Kitis, N. Vlachos, General semi-analytical expressions for TL, OSL and other luminescence stimulation modes derived from OTOR model using the Lambert W function, *Radiat. Meas.* 48 (2013) 47–54.
- [30] L. Lovedy Singh, R.K.K. Gartia, Theoretical derivation of a simplified form of the OTOR/GOT differential equation, *Radiat. Meas.* 59 (2013) 160–164.
- [31] R.M. Corless, D.J. Jeffrey. *The Wright  $\omega$  Function Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)* vol. 2385, pp. 76–89 21.