



On the resolution of overlapping peaks in complex thermoluminescence glow curves

George Kitis^{a,*}, Vasilis Pagonis^b

^a Aristotle University of Thessaloniki, Physics Department, Nuclear Physics and Elementary Particles Physics Section, 54124 Thessaloniki, Greece

^b McDaniel College, Physics Department, Westminster, MD 21157, USA

ARTICLE INFO

Keywords:

Thermoluminescence
Resolution
TL peak overlap
TL glow curve deconvolution
TL curve fitting

ABSTRACT

Experimental Thermoluminescence (TL) glow curves for most dosimetric materials are composites, consisting of weakly or strongly overlapping peaks. The ability to discriminate between two overlapping peaks defines the resolution of a TL glow curve. Although the concept of resolution has been defined and used widely in many areas of science, there have been no previous attempts to define and study the resolution of overlapping TL peaks. In this work the resolution parameter R is defined in terms of the geometrical characteristics of TL peaks. A large number of TL glow curves consisting of two peaks were numerically evaluated for various degrees of overlapping between them. These numerically generated glow curves were analyzed by a computerized glow curve deconvolution analysis, in order to determine the reliability of the deconvolution results as a function of the resolution parameter R .

1. Introduction

Thermoluminescence (TL) finds extended applications in radiation dosimetry and in archaeological and geological dosimetric methods of dating. An experimental thermoluminescence (TL) glow curve consists of several either weakly or strongly overlapping TL glow peaks. The cornerstones of practical applications of TL are (a) the functional relation of TL with the radiation dose and (b) the stability of TL signal over long periods of time. Both of these factors have been researched extensively, with the aim of providing dosimetric characterization and energy level characterization [1–3]. The aim of both characterizations is to obtain the most suitable part of the TL glow curves during practical applications.

TL signals are analyzed by measuring either the peak height at specific temperatures, or as an integrated signal between two preselected temperatures. When overlapping exists between TL peaks, the accuracy of both methods is greatly decreased [1].

An alternative method is to analyze the complex TL glow curve into its individual TL peaks by using a computerized glow curve deconvolution (CGCD) analysis [4]. This method can provide both a clear estimate of the TL signal, as well all the data needed to evaluate theoretically the stability of the TL signal over long periods of time, and is used widely for many dosimetric materials.

The easiest part of a CGCD analysis is to achieve a very good fit to the experimental glow curves, but the most crucial and difficult part of the analysis is to interpret the results correctly. When the experimental TL glow curve contains strongly overlapping peaks, care must be taken

to apply the CGCD analysis correctly. The reliability of the CGCD and therefore of its correct interpretation is closely correlated with the degree of overlapping of the individual TL peaks. It is then important to find suitable criteria for defining and evaluating the resolution of overlapping TL peaks. An attempt to develop such criteria for linearly modulated optically stimulated luminescence signals (LM-OSL) was carried out by Kitis and Pagonis [5]. These authors found that it is possible to distinguish between two overlapping LM-OSL peaks if the times at the maximum intensity of LM-OSL curves differ by at least 15%.

Although the concept of peak resolution has been defined and used widely in many areas of science, there have been no previous attempts in the literature to define and study the resolution of overlapping TL peaks.

The main goals of the present work are

- To define the resolution factor R of two closely overlapping TL peaks, in terms of the well-known geometrical properties of TL peaks,
- To investigate the dependence of R on the temperature separation and the intensity of the TL peaks, and
- To investigate the impact of the magnitude of the resolution R on the ability of CGCD analysis to give reliable results.

2. Resolution - definition

In many fields of physics experimental results are obtained in the form of a spectrum consisting of several individual peaks, which can be:

* Corresponding author.

E-mail address: gkitis@auth.gr (G. Kitis).

(a) well separated (b) weakly overlapping and (c) strongly overlapping. Due to the highly informative nature of each peak, complex spectra are subjected to computerized analysis with the aim of separating the overlapping peaks and obtaining the relevant information. The degree of overlapping between peaks is called resolution, and is formulated in this section in terms of the geometrical characteristics of the peaks.

A TL peak is characterized by the temperatures at the peak maximum intensity T_m and the two temperatures at the half maximum intensity $T_1 < T_m$ and $T_2 > T_m$. These temperatures further define the relevant widths quantities $\omega = T_2 - T_1$, $\tau = T_m - T_1$ and $\delta = T_2 - T_m$ [1–3,6]. Fig. 1 shows three different situations of two overlapping peaks; the degree of overlap depends on the quantity δ_1 of the lower temperature peak and the quantity τ_2 of the high temperature peak. By following the methods used for high resolution chromatography [7,8], we quantify the degree of overlapping by the quantity R defined as:

$$R = \frac{T_{m2} - T_{m1}}{\delta_1 + \tau_2} \quad (1)$$

The value of R depends on the parameter $x = (T_{m2} - T_{m1}) - (\delta_1 + \tau_2)$ shown in Fig. 1. In the situation shown in Fig. 1(a), the quantity x represents the part of $(T_{m2} - T_{m1})$ which does not belong to the two peaks, and this defines a resolution R given by:

$$R = \frac{T_{m2} - T_{m1}}{\delta_1 + \tau_2} = \frac{x + \delta_1 + \tau_2}{\delta_1 + \tau_2} = 1 + \frac{x}{\delta_1 + \tau_2} \quad (2)$$

Therefore in the case shown in Fig. 1(a), the quantity x is such that the resolution $R > 1$.

In the case shown in Fig. 1(b) the parameter $x = (T_{m2} - T_{m1}) - (\delta_1 + \tau_2) = 0$, and this defines a resolution $R = 1$:

$$R = \frac{T_{m2} - T_{m1}}{\delta_1 + \tau_2} = 1 \quad (3)$$

In the case of Fig. 1(c) x represents the part of $(T_{m2} - T_{m1})$ which is common to both peaks. In this case, one obtains a resolution $R < 1$, since $x = (\delta_1 + \tau_2) - (T_{m2} - T_{m1})$ and therefore:

$$R = \frac{T_{m2} - T_{m1}}{\delta_1 + \tau_2} = \frac{\delta_1 + \tau_2 - x}{\delta_1 + \tau_2} = 1 - \frac{x}{\delta_1 + \tau_2} \quad (4)$$

When $T_{m2} = T_{m1}$ the overlapping of the two TL peaks is absolute, and this corresponds to a resolution $R = 0$.

Since most of the readers are familiar with the full width of a TL peak denoted by the full width at half maximum ω , Eq. (1) can also be written for the sake of simplicity in terms of ω . By using the approximation

$$\delta_1 + \tau_2 \approx \omega_1 \text{ or } \approx \omega_2 \quad (5)$$

the resolutions can be defined in terms of ω as:

$$R = \frac{T_{m2} - T_{m1}}{\omega_1 \text{ (or } \omega_2)} \quad (6)$$

3. Evaluation of synthetic TL glow curves

In the present study the TL glow peaks will be numerically derived using the general order kinetics equation by May and Partridge [9].

$$I(n_0, E, s, b, T) = n_0^b s'' e^{-\frac{E}{kT}} \left[1 + \frac{(b-1)s''}{\beta} \int_{T_0}^T e^{-\frac{E}{kT'}} dT' \right]^{-\frac{b}{b-1}} \quad (7)$$

where $s'' = s' n_0^{b-1}$ is the frequency factor for general order kinetics, n_0 (cm^{-3}) is the initial concentration of filled electron traps, E (eV) is the activation energy, b the kinetic order parameter with a value usually between 1 or 2, s' ($\text{m}^{3(b-1)} \text{s}^{-1}$) the pre-exponential factor and T (K) is the temperature. It is noted that this is an empirical equation which has been found useful in representing adequately experimental TL glow curves in various materials.

By considering Eq. (7) for $T = T_m$ we obtain

$$I_m = n_0^b s'' e^{-\frac{E}{kT_m}} \left[1 + \frac{(b-1)s''}{\beta} \int_{T_0}^{T_m} e^{-\frac{E}{kT'}} dT' \right]^{-\frac{b}{b-1}} \quad (8)$$

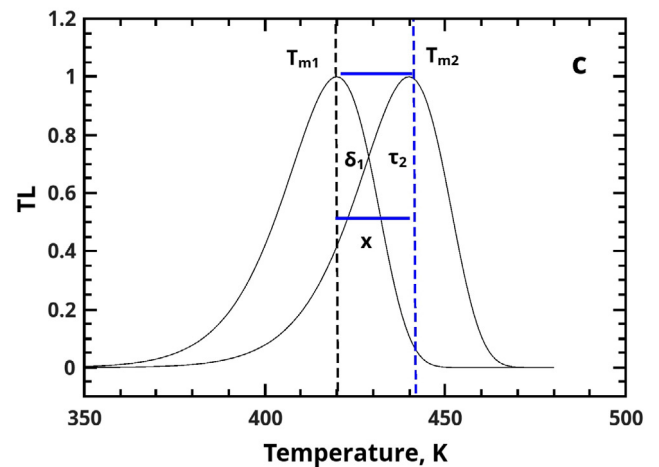
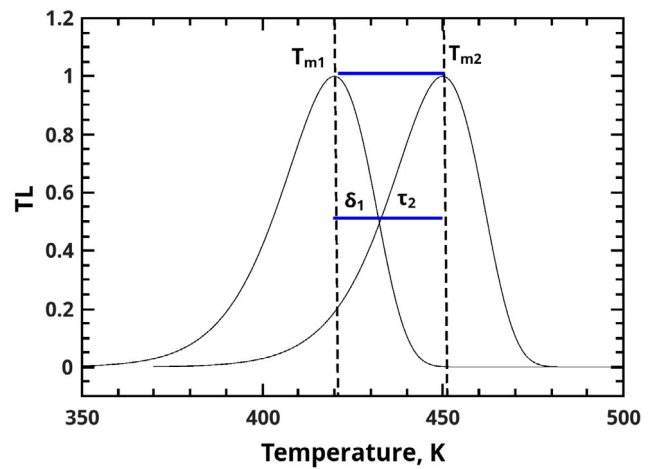
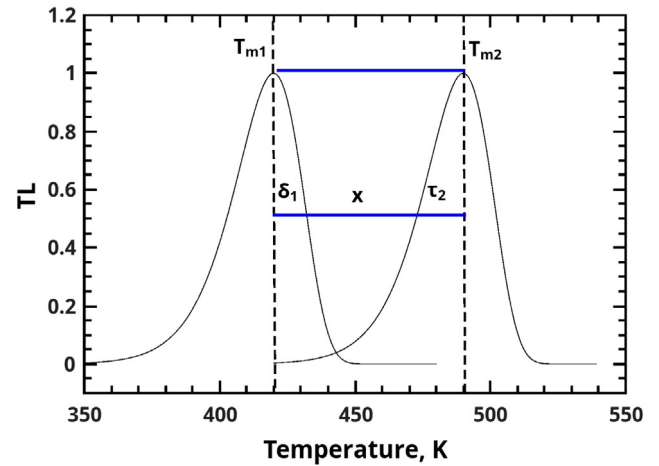


Fig. 1. Example of two-peak TL glow curve, showing the definition of the resolution factor R .

where I_m is the maximum TL intensity.

The condition for maximum TL intensity is found by equating the derivative of Eq. (7) to zero, to obtain [1,2]:

$$1 + \frac{(b-1)s''}{\beta} \int_{T_0}^{T_m} e^{-\frac{E}{kT}} dT = \frac{b s'' n_0^{b-1} k T_m^2}{\beta E} e^{-\frac{E}{kT_m}} \quad (9)$$

The exponential integral appearing in Eq. (7) is usually approximated by a asymptotic series approximation which is valid only for $E > 14kT$. For $E < 14kT$ the exponential integral is approximated by a power series [10]. However, in modern software this is not necessary because, due to its importance and generality, the exponential integral function is implemented as a built-in function like the common sine, cosine etc. Therefore, the exponential integral in Eqs. (7)–(8) can be evaluated by the following equations:

$$F(E, T) = \int_{T_0}^T e^{-\frac{E}{kT'}} dT' = T e^{-\frac{E}{kT}} + \frac{E}{k} Ei\left[-\frac{E}{kT}\right] \quad (10)$$

$$F(E, T_m) = \int_{T_0}^{T_m} e^{-\frac{E}{kT'}} dT' = T_m e^{-\frac{E}{kT_m}} - \frac{E}{k} Ei\left[-\frac{E}{kT_m}\right] \quad (11)$$

Eq. (7) was transformed by Kitis et al. [11], in the more useful form of $I(I_m, E, T_m, b, T)$. However, according to above discussion about the exponential integral function, the equation proposed by Kitis et al. [11] can be slightly modified in order to use the built-in exponential integral function. The algebra needed to obtain the modified version of the original equation by Kitis et al. [11] is as follows:

- Divide Eq. (7) over Eq. (8), to eliminate the values of s'' and n_0^b
- Use the condition for the maximum Eq. (9), to eliminate the values of s'' and β
- Use Eqs. (10) and (11) for the integral appearing in Eqs. (7) and (8).

After the above simple algebra steps, the modified form of the original equation by Kitis et al. [11] is:

$$I(T) = I_m e^{\left[-\frac{E}{kT} \cdot \frac{T_m - T}{T_m}\right]} \cdot \left[1 + \frac{b-1}{b} \frac{E}{kT_m^2} e^{\frac{E}{kT_m}} \{F(E, T) - F(E, T_m)\}\right]^{-\frac{b}{b-1}} \quad (12)$$

The composite TL glow curves, which are numerically derived using Eq. (7) have to be analyzed by a computerized glow curve deconvolution (CGCD) procedure using the above Eq. (12) along with Eqs. (10) and (11).

4. Study of numerical TL glow curves

This section describes three sets of synthetic glow curves consisting of two partially overlapping peaks. In the first set, the robustness of the resolution R , is demonstrated by showing that it depends rather weakly on the kinetic parameters E, s, b . In the second and third set of synthetic glow curves, we examine how the resolution R affects the accuracy of the commonly used CGCD procedures.

4.1. Synthetic set #1: Dependence of the resolution R on the kinetic parameters E, s, b

According to its definition by Eq. (1), the resolution R depends on the geometrical factors ω, τ and δ . One of the characteristics of TL peaks is that at each temperature T_m correspond an infinite number of E, s, b values. This situation is very different from the analysis of LM-OSL signals, where to each time maximum corresponds one and only one LM-OSL peak [5]. Therefore, our study has to take into account this fact, and we must investigate its impact on the resolution parameter R .

In a first set we study the dependence of R on the following three factors:

- The parameters E, s (for a fixed kinetic order b)
- The distance $\Delta T_m = T_{m2} - T_{m1}$ between the two peaks and
- The kinetic order parameter b .

In these synthetic set the position of the first peak is fixed at $T_{m1} = 420$ K, and the position of the second peak is varied in the range 420–470 K in steps of 10 K. The heights of the two TL peaks are taken to be the same. For each fixed temperature T_{m1} and T_{m2} , a large number of E, s pairs is evaluated which produces a TL peak with the same temperature T_m . This is achieved according to the following protocol.

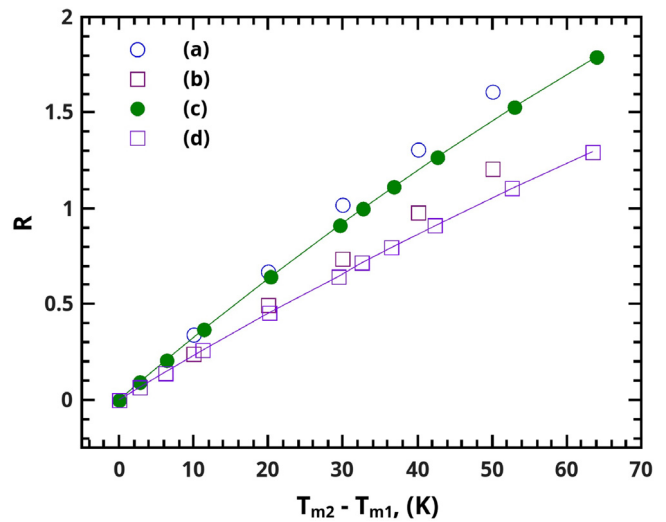


Fig. 2. Resolution R as a function of the difference $T_{m2} - T_{m1}$ for a large number of (E, s) pairs. (a) First order kinetics (b) second order kinetics. (c), (d) For first and second order kinetics peaks with $E = 1$ eV and s varying from 10^{10} to 10^{12} s $^{-1}$.

Table 1

Values of R as a function of ΔT_m for first order (F.O) and second order (S.O). Mean values from 40–50 E, s pairs.

ΔT_m (K)	R (F.O)	R (S.O)
10	0.34 ± 0.07	0.24 ± 0.05
20	0.67 ± 0.10	0.50 ± 0.09
30	1.02 ± 0.16	0.74 ± 0.13
40	1.31 ± 0.21	0.98 ± 0.16
50	1.61 ± 0.27	1.21 ± 0.21

- step 0: We use only first order kinetics for both TL peaks ($b = 1.0001$ in Eq. (7)), and select a fixed position of the first peak at $T_{m1} = 420$ K.
- step 1: Select a temperature $T_{m2} = 430$ K for the second peak.
- Step 2: Evaluate all pairs of E in the region (0.8–2 eV) and s in the region ($10^8 - 10^{20}$ s $^{-1}$) which result in the same T_{m2} for the second TL peak in step 1. This results in a total number of 40–50 E, s pairs, for each kinetic order studied.
- Step 3: For each TL glow peak and for each E, s pair, evaluate the quantities ω, τ, δ and calculate the resolution R using Eq. (1).
- Step 4: Apply steps 1 to 3 for $T_{m2} = 430, 440, 450, 460$ and 470 K, in order to study the effect of the peak separation $\Delta T_m = T_{m2} - T_{m1}$ on the resolution R .

Typical results of the procedure in this section are shown in Fig. 2 and Table 1, and are discussed in the Results section of his paper.

The complete set of synthetic glow curves in steps 0–4 above are then repeated for the case of second order kinetics ($b = 2$), in order to see the effect of the kinetic order b on the resolution R . We decided to study only the cases of first and second order kinetics, because they are the limiting cases of single TL peaks, with symmetry factor $0.42 < \mu_g = \delta/\omega < 0.52$ [2,6].

4.2. Simulation set #2: Dependence of the accuracy of CGCD on R , for TL peaks of different s values

In a second set of synthetic TL curves, CGCD is used to analyze a system of two TL peaks with different s values as follows:

- Step 1: Two single TL peaks were selected with the same values of n_0 , and with the parameters $E_1 = E_2 = 1$ eV, $s_1 = 10^{12}$ s $^{-1}$.
- Step 2: The E_1, s_1 values of the first peak and the E_2 value of the second peak are kept constant.

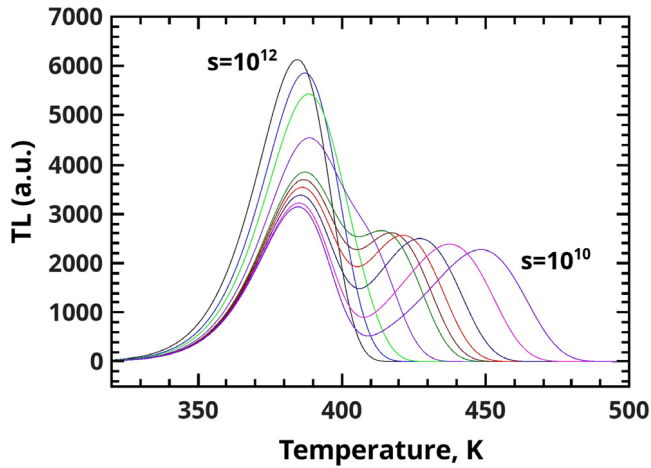


Fig. 3. Series of numerical TL glow curves consisting of two peaks derived according to second method.

- Step 3: The value of s_2 is gradually decreased from 10^{12} to 10^{10} s^{-1} . This causes a shift of the second peak to higher temperatures, and separates gradually the two peaks along the temperature axis.
- Step 4: The resolution R is evaluated from the values of T_m , ω , δ_1 and τ_2 according to Eq. (1).
- Step 5: The TL glow curves of step 4 are subjected to CGCD analysis.

Typical examples of these synthetic curves are shown in Fig. 3. It is noted that similar results are obtained when the value of s_2 is kept constant, and the value of E_2 is increased instead.

4.3. Simulation set #3: Dependence of the accuracy of CGCD on R , for TL peaks of unequal heights

In this section we describe a third set of synthetic glow curves, in which CGCD is used to analyze a system of two TL peaks derived by using the same set of trapping parameters used in Section 4.1. The resolution R is studied as a function of the temperature difference $\Delta T_m = T_{m2} - T_{m1}$, as well as a function of the relative intensities of the two TL peaks (for fixed value of ΔT_m). The details of the study are as follows:

- Step 1: TL peaks were derived with E, s values corresponding to ΔT_m equal to 10, 20, 30, 40 and 50 K.
- Step 2: The areas of the two TL peaks are initially taken to be equal, by choosing the same parameter n_0 . Then the TL integral of the first peak was kept constant, whereas the peak integral of the second peak was decreased by the factors $1 n_0, 0.8 n_0, 0.6 n_0, 0.4 n_0, 0.2 n_0, 0.1 n_0$. Six different TL glow curves are produced in this manner, with typical results shown in Figs. 4–5.
- Step 3: The TL glow curves of step 2 were subjected to CGCD analysis.

5. CGCD analysis, goodness of fit and initial parameter values

All synthetic TL glow curves obtained by the methods described above were subjected to CGCD analysis using Eq. (12). In the present work the ROOT data Analysis Framework was used [12]. All fittings were performed using the MINUIT program [13] released in ROOT, which is a physics analysis tool for function minimization. The exponential integral function, $E[i]$ is implemented in ROOT through the GNU scientific library (GNU GSL) [14].

The goodness of fit was tested using the figure of merit (FOM) [15] which is given by

$$FOM = \sum_i \frac{|Y_E - Y_F|}{A}, \quad (13)$$

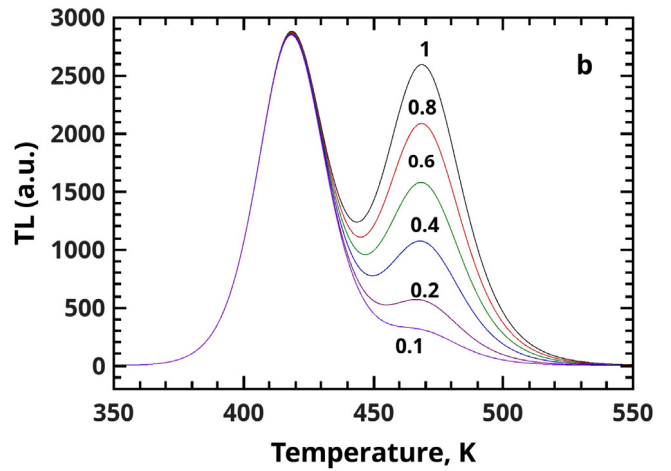
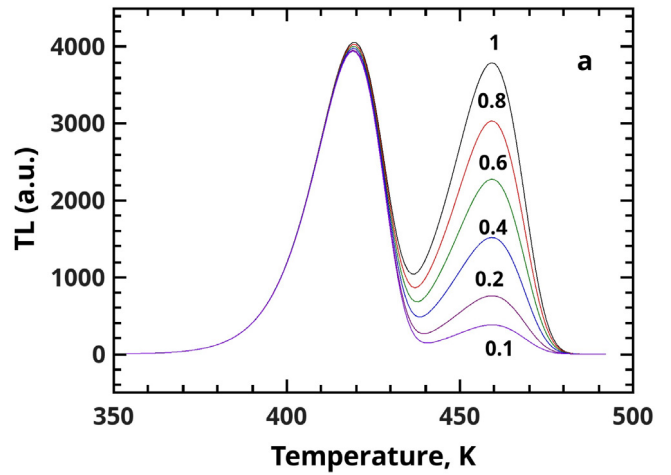


Fig. 4. Examples of numerically evaluated TL glow curves consisting of two peaks with $T_{m2} - T_{m1} = 40 \text{ K}$ and a resolution $R > 1$. (a) First order and (b) Second order kinetics.

where Y_E are the points in the synthetic glow-curve, Y_F are the corresponding points in the fitted glow curve using the CGCD procedure, and A is the area of the fitted glow-curve.

6. Results and discussion

6.1. Results from synthetic set #1

The resolution values R evaluated using the synthetic single TL peaks as described in Section 4.1 are listed in Table 1. Every value of R is the mean and standard deviation from 40–50 (E, s) pairs. The same results are also plotted in Fig. 2, along with resolution results of protocol in Section 4.2, which are discussed later in this paper. It is clear that there is very good agreement between the resolution R values evaluated from the TL peaks using both methods.

From Fig. 2 it is clear that in general the resolution is better for first order kinetics, and this is evident more clearly for $\Delta T_m > 20 \text{ K}$. However, for $R > 0.5$ it seems that the value of R does not impact the CGCD analysis, despite the differences existing between first and second order kinetics. This, however, has to be confirmed by the results of the CGCD analysis, which will be presented in the next section.

6.2. Extraction of peak parameters from the CGCD procedure

When the CGCD analysis is applied to experimental glow curves, the initial guess values of the free parameters used in the algorithm are

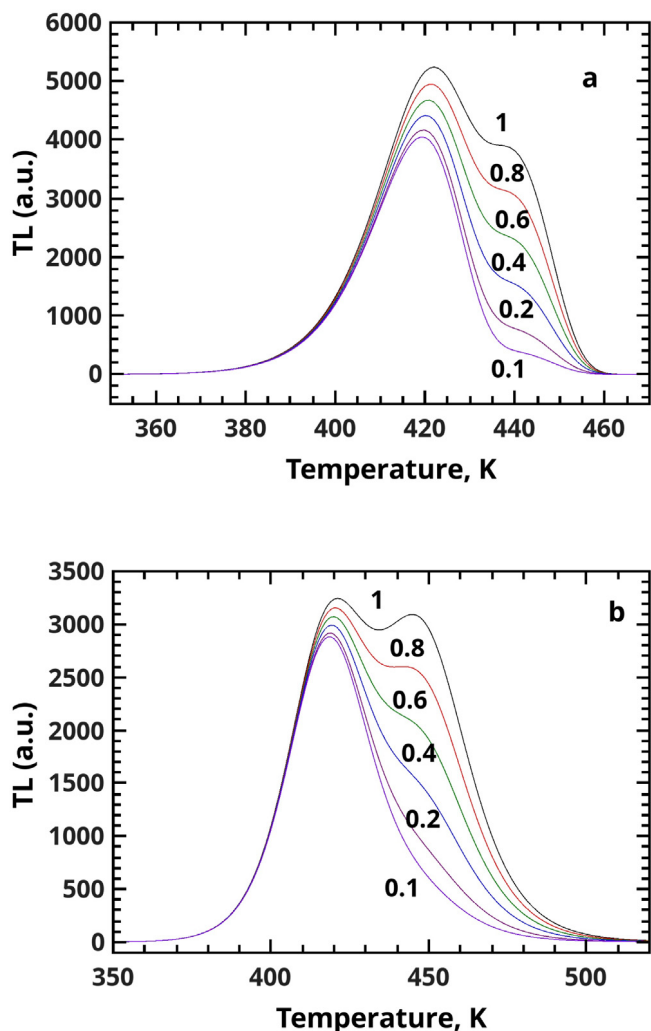


Fig. 5. Examples of numerically evaluated TL glow curves consisting of two peaks with $T_{m2} - T_{m1} = 20$ K, and a resolution $R = 0.85$. (a) Results for first order and (b) for second order kinetics.

extremely important. Therefore, a separate method of analysis like the initial rise method is used to evaluate the values of activation energies E to be used as input in the CGCD algorithms.

The TL analytical Eq. (12) is of the form $I(I_m, E, T_m, b, T)$, and the values of the free parameters I_m and T_m can be extracted from the experimental glow curves with high accuracy.

Although the exact values of the parameters E , s , b of synthetic curves are known in this paper, we use the following CGCD procedure to obtain unbiased results. Four parameter values are used as input to the MINUIT program. These 4 parameters are the initial guess value, its estimated error, its lowest possible limiting value and its maximum possible limiting value. For example, the activation energy of all peaks starts with a guess value of 1 eV and an error of 0.1 eV, with the lower limit value set 0.8 eV, and the upper limit value set 2 eV. The T_m values of the peaks start with a guess value of 390 K, and lower and upper limits at 370 K and 470 K correspondingly. The I_m limits vary from 0 to 10^4 a.u., and the kinetic order b limits are set from $b = 1.0001$, up to $b = 2.1$. Using this methodology it is very probable to achieve an unbiased fitting procedure.

6.3. Results from synthetic set #2

Fig. 3 shows the sequence of the numerically evaluated first order TL glow curves using the second method described in Section 4.2. The

Table 2
CGCD analysis of glow curves in Fig. 7 using one TL peak component.

T_m (K)	E (eV)	FOM%
384.5	1	0.0001
385.8	0.98	0.02
387.7	0.96	1.7
390	0.90	5.5

resolution values as a function of peak separation are shown in Fig. 2, and the FOM values from CGCD analysis were better than 0.001%. However, despite these excellent FOM values the CGCD results are not correct when the glow curves shape has the shape of single peak.

The single peak like glow curves were also analyzed using one peak component. The results are shown in Table 2. The first row corresponds to $R = 0$ and to the absolute degeneration case. However, the quality of fit indicated by the FOM values drops quickly, as the activation energy E is varied. The FOM value of 4.6% for a $\Delta T_m = 6$ K, which is already unacceptable.

The results of Fig. 2(b) and of Table 2 are very important, because they give researchers a criterion which can be used to determine whether an experimental glow curve is composite or not.

6.4. Results from synthetic set #3

Cases with resolution $R > 1$

Fig. 4 shows TL glow curves generated using the protocol in Section 4.3, with a resolution of $R > 1$. The TL glow curves shown in Fig. 4(a) and (b) are obtained for first and second order kinetics, correspondingly. This is an example of weakly overlapping peaks. The intensity of the first peak is stable, whereas the intensity of the second vary following the fractions shown in the figure. All TL glow curves were analyzed by CGCD analysis, and the FOM values were better than 0.4%.

The comparison of the *input* parameters in the synthetic curves in Fig. 4, and the *output* parameters extracted from the CGCD procedure are presented here in the form [input, output \pm error] as follows:

• First order kinetics

1. Peak 1: The output values of first peak were exactly equal to the input values
2. Peak 2: T_m [460, 459 \pm 0.35], E [1.8, 1.83 \pm 0.04] and b [1.0001, 1.01 \pm 0.01].

• Second order

1. Peak 1: T_m [420, 418.3 \pm 0.04], E [1.65, 1.654 \pm 0.004] and b [2, 2.03 \pm 0.01].
2. Peak 2: T_m [470, 69.2 \pm 0.25], E [1.85, 1.87 \pm 0.03] and b [2, 2.003 \pm 0.002].

These results show that for cases with resolution of $R > 1$, the CGCD overall performs in an ideal way, and reproduces the input parameters very accurately.

Cases with resolution $1 > R > 0.5$

Fig. 5(a) and (b) shows additional examples of numerically evaluated TL glow curves with a resolution of $R = 0.85$. The examples shown consist of two TL peaks with first order kinetics in (a), and with second order kinetics in (b). This is an example of strongly overlapping peaks. The CGCD was satisfactory, with FOM values better than 0.1% for all TL curves in the figure.

The comparison of the *input* parameters in the synthetic curves in Fig. 5, and the *output* parameters extracted from the CGCD procedure in the same form [input, output \pm error] are as follows.

• First order kinetics

1. Peak 1: T_m [420, 419 \pm 0.5], E [1.55, 1.56 \pm 0.02]

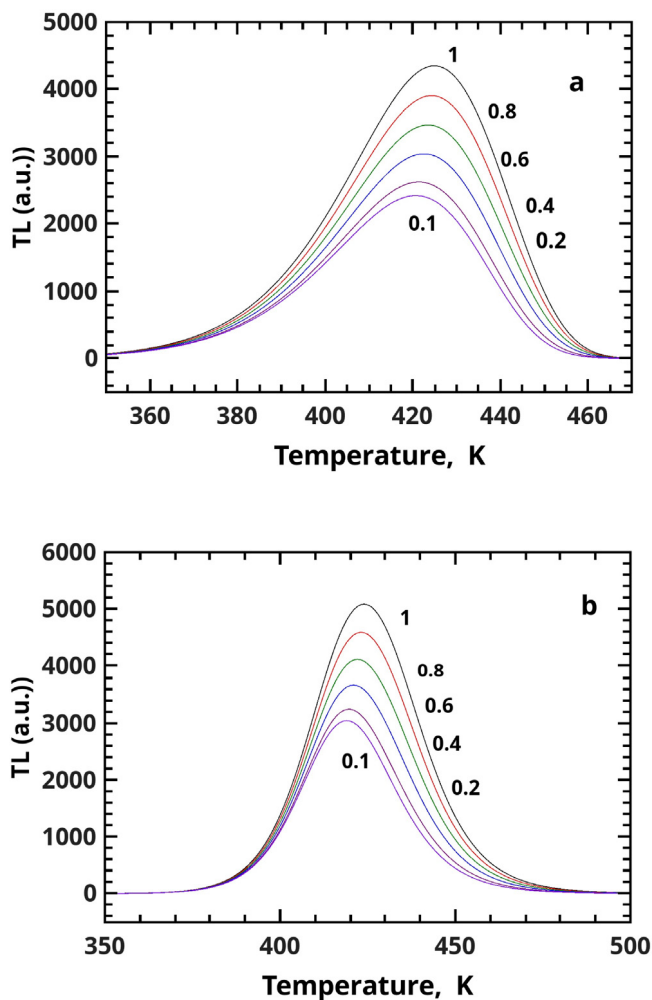


Fig. 6. Examples of numerically evaluated TL glow curves consisting of two peaks with $T_{m2} - T_{m1} = 10$ K. Left hand side for first order and right hand side for second order kinetics.

2. Peak 2: T_m [440, 438.9 ± 0.3], E [1.65, 1.675 ± 0.003] and b [1.0001, 1.008 ± 0.001].

• Second order kinetics

1. Peak 1: T_m [420, 418.3 ± 0.1], E [1.65, 1.655 ± 0.008] and b [2, 2.014 ± 0.01].

2. Peak 2: T_m [450, 448.7 ± 0.85], E [1.75, 1.76 ± 0.07] and b [2, 2.006 ± 0.002].

Cases with resolution $R < 0.5$

Finally Fig. 6(a) and (b) shows examples of numerically evaluated TL glow curves of first and second order kinetics, with a resolution of $R = 0.25$. Obviously this is an example of strongly overlapping peaks. From the point of view of FOM, the CGCD was quite satisfactory with FOM values better than 1% for all TL curves in this figure.

The overlapping of individual theoretical peaks in glow curves of Fig. 6 is so strong, that the whole composite glow curves has the shape of a single TL peak. When the CGCD analysis was applied on these glow curves using a single glow peak, the FOM was still excellent and better than 0.01%. Examples of two peak and one peak analysis are shown in Fig. 7. It is easily seen that the fit is very good, but both analyses are erroneous.

When using the two peak analysis, the T_m and E values were close to the input values, for both first and second order kinetics. However, the results were erroneous because the order of peaks is the opposite of

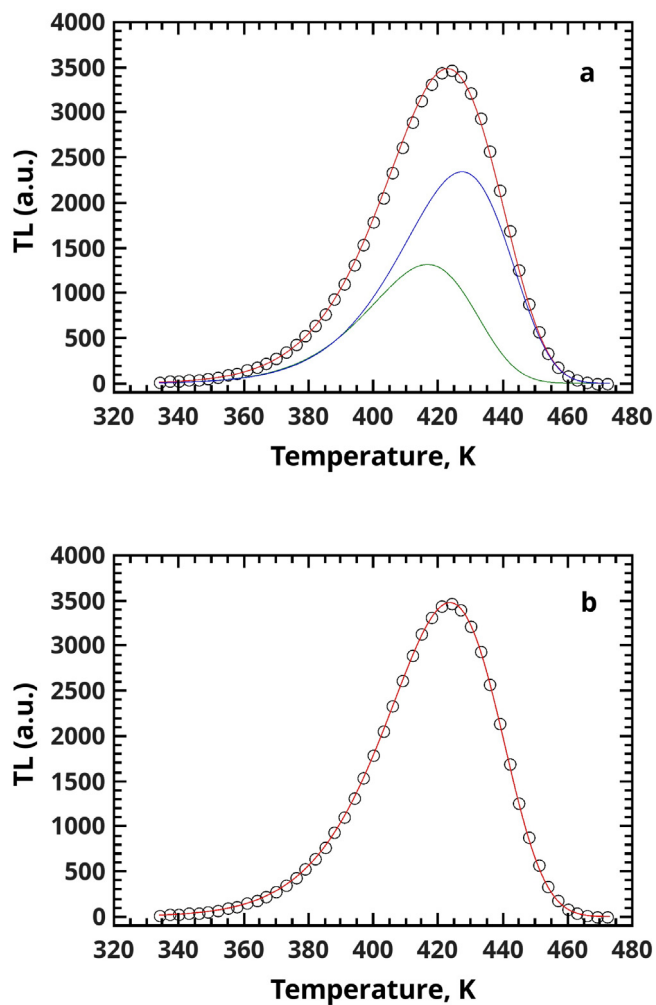


Fig. 7. Fitting example for a degenerated case. The single like peak is composite consisting of two peaks with $T_{m2} - T_{m1} = 10$ K, and a resolution $R = 0.25$. (a) Results for first order and (b) for second order kinetics. The fit using two components gave FOM=1.2%, whereas the fit using one component gave FOM = 0.4%. Despite the very good FOM, both deconvolution results are erroneous.

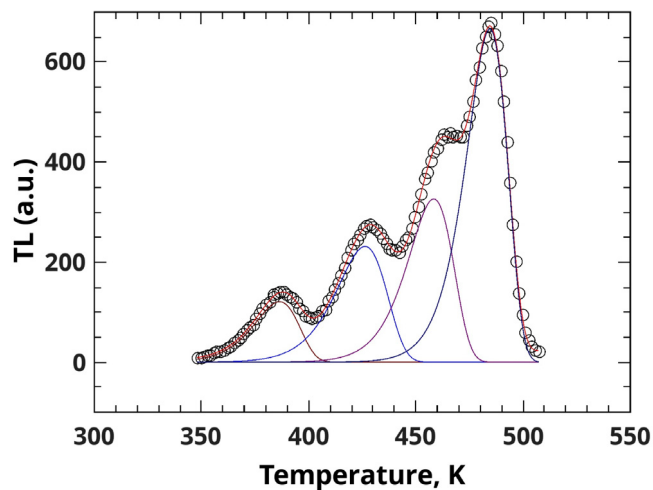


Fig. 8. CCGD analysis of the REFGLOW003 of the GLOCANIN project, which is an experimental glow peak, in order to evaluate the resolution among its individual peaks.

Table 3

Evaluation of resolution among peaks of glow curves LiF:Mg,Ti after the analysis of its glow curves using a CGCD procedure.

Peqak	T_m (K)	ω (K)	Resolution
2	386.4	25.4	–
3	426.3	28.1	$R_{23} = 1.40 - 1.60$
4	458.3	25.6	$R_{34} = 1.12 - 1.28$
5	484.5	23.2	$R_{45} = 1.02 - 1.13$

that expected. Namely, the second component peak had to be smaller by construction, but the opposite was found during the CGCD analysis. In other words, the arrangement of the two peaks in CGCD was random, without any relation to the initial values of n_0 .

When using a single peak analysis, the T_m and E values were again close to the input values, for both first and second order kinetics. Specifically the results were:

- First order: Input T_m 420 and 430 K. Output $T_m = 423 \pm 1.8$. Input E values 0.85 and 0.95. Output $E = 0.86 \pm 0.04$
- Second order: Input T_m 420 and 430 K. Output $T_m = 422 \pm 1.9$. Input E values 1.65 and 1.7. Output $E = 1.57 \pm 0.04$ and $b = 1.99 \pm 0.01$.

However, this single peak analysis is obviously also erroneous, and the results of the CGCD are meaningless.

6.5. A practical example using LiF:Mg,Ti

LiF:Mg,Ti is the most common TL dosimeter, so it is selected as a practical example for evaluation of the resolution among its individual peaks. The glow curve chosen was taken from the collection of the reference glow curves of the GLOCANIN inter comparison program by Bos et al. [16,17]. The REFGLOW003, which is an experimental glow curve containing the glow peaks 2, 3, 4 and 5 of LiF:Mg,Ti after a 15 mGy ^{60}C dose. The glow curve was analyzed using Eq. (12) along with Eqs. (10) and (11). The values of the kinetic order used was $b = 1.00001$ for which the general order equations gives exactly the first order kinetics. The kinetic parameters E and s found are the same with that of the GLOCANIN project. The resolution was evaluated among the peaks 2 and 3 R_{23} , the peaks 3 and 4 R_{34} and the peaks 4 and 5 R_{45} . The resulting values are listed in Table 3. The resolution values are all greater than 1. These values are very satisfactory and ensure the reliability of the results of the CGCD analysis of the glow curve of LiF:Mg,Ti (see Fig. 8).

7. Discussion- general resolution criteria

From the results presented above, it becomes clear that the problems in TL analysis due to resolution appear for $R < 0.5$. Following the aim of the present work it is useful to define regions of R , which will be related with reliability of CGCD analysis as follows.

- $R > 1$: This case represents isolated or weakly overlapping peaks. The results of the CGCD analysis are obviously reliable.
- $0.5 < R < 1$: This case represents strong overlapping between two peaks. The results of the CGCD are obviously not reliable, but they

can be made reliable by using additional TL methods for trapping parameter evaluation.

- $0.25 < R < 0.5$: This case represents extremely strong overlapping. The sum of two peaks tend to take the shape of a single peak. Their analysis with CGCD is possible, but its reliability will depend on additional TL measurements.
- $0 < R < 0.25$: In this region the sum of the two peak already has the shape of a single peak. The CGCD analysis is able to identify the complex nature of the single shaped glow curve, but it is not able to give a uniquely reliable solution. This can be achieved only by the combination of CGCD analysis with other TL methods.
- $R \approx 0$: Represents the absolute degeneration case, where CGCD analysis is meaningless without additional experiments or additional analysis.

8. Conclusions

The conclusions of the present work can be summarized as following:

- The CGCD analysis can always achieve a very good fit to any glow curve, however this does not mean that the CGCD results are always reliable.
- The resolution R is defined quantitatively in the present work, and can help researchers estimate the reliability of the CGCD analysis.
- For resolution of $R > 0.5$ which corresponds to peak maximum temperature difference $T_{m2} - T_{m1}$ greater than the full width ω of the peaks, the CGCD results are always reliable.
- For resolution $0.25 < R < 0.5$ which corresponding to peak maximum temperature difference $T_{m2} - T_{m1}$ less than the full width ω , the two-peak glow curve appears as a single TL peak. The CGCD can give reliable results, but only in combination with other TL methods.
- For resolution $R < 0.25$ the results of the CGCD analysis are meaningless.

References

- [1] R. Chen, Y. Kirsh, *Analysis of Thermally Stimulated Processes*, Pergamon Press, 1981.
- [2] R. Chen, S.W.S. McKeever, *Theory of Thermoluminescence and Related Phenomena*, World Scientific, 1997.
- [3] V. Pagonis, G. Kitis, C. Furetta, *Numerical and Practical Exercises in Thermoluminescence*, Springer, 2006.
- [4] Y.S. Horowitz, D. Yossian, *Radiat. Prot. Dosim.* 60 (1995) special issue.
- [5] G. Kitis, V. Pagonis, *Radiat. Meas.* 43 (2008) 737.
- [6] G. Kitis, V. Pagonis, *Nucl. Instrum. Methods Phys. Res. B* 262 (2007) 313.
- [7] John W. Dolan, 2002. <http://www.chromatographyonline.com/peak-tailing-and-resolution-1>.
- [8] P. Sandra, *High Resol. Chromatography* 12 (1989) 82.
- [9] C.E. May, J.A. Partridge, *J. Chem. Phys.* 40 (1964) 1401.
- [10] G. Kitis, R. Chen, V. Pagonis, E. Carinou, V. Kamenopoulou, *J. Phys. D: Appl. Phys.* 39 (2006) 1500.
- [11] G. Kitis, J. Gomez Ros, J.W.N. Tuyn, *J. Phys. D: Appl. Phys.* 31 (1998) 2636.
- [12] ROOT, A data Analysis Framework, <https://root.cern.ch>.
- [13] MINUIT, A physics analysis tool for function minimization. Released in ROOT.
- [14] GSL-GNU Scientific Library, www.gnu.org/software/gsl.
- [15] H.G. Balian, N.W. Eddy, *Nucl. Instrum. Methods* 145 (1977) 389.
- [16] A.J.J. Bos, T.M. Piters, J.M. Gomez Ros, A. Delgado, *Radiat. Prot. Dosim.* 51 (1993) 257–264.
- [17] A.J.J. Bos, T.M. Piters, J.M. Gomez Ros, A. Delgado, *Radiat. Prot. Dosim.* 47 (1994) 473–477.