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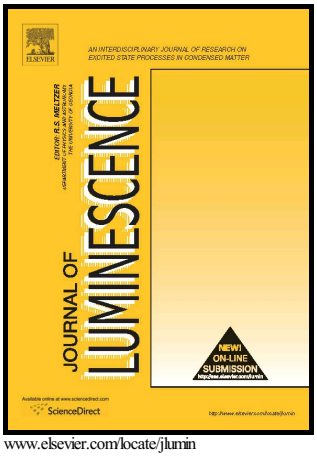

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On the analysis of glow curves with the general order kinetics: reliability of the computed trap parameters

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Abstract
Nowadays the most employed kinetics for analyzing glow curves is the general order kinetics (GO) proposed by C. E. May and J. A. Partridge. As shown in many articles this kinetics might yield wrong parameters characterizing trap and recombination centers. In this article this kinetics is compared with the modified general order kinetics put forward by M. S. Rasheedy by analyzing synthetic glow curves. The results show that the modified kinetics gives parameters, which are more accurate than that yield by the original general order kinetics. A criterion is reported to evaluate the accuracy of the trap parameters found by deconvolving glow curves. This criterion was employed to assess the reliability of the trap parameters of the YVO_4: Eu^{3+} compounds.

Introduction
Glow curve analysis is a frequently used procedure for investigating the kinetics involved in thermoluminescence (TL). Basically it relies on choosing a model, which is in accordance with experimental results at hand, and on deriving a theoretical expression for the emitted light $I_{th}(T,\alpha)$ (glow curve) from the set of differential equations describing the carrier traffic among traps and recombination centers. T stands for the temperature, and α for the set of parameters characterizing traps and recombination centers. The simplest model, known as one trap-one recombination center (OTOR), is shown in figure 1.

Fig. 1: OTOR model. A_m is the recombination probability, h is the concentration of holes in the recombination center, A_n is the retrapping probability, N is the concentration of traps, n is the concentration of trapped electrons, s is the frequency factor, E the activation energy, and k is the Boltzmann constant. The product s·exp(-E/kT) is the escape probability of an electron from a trap.

For the model shown in figure 1 the set of parameters is $\alpha = [E, s, n0, A_m, A_n]$, where n_0 stands for the initial concentration of trapped electrons. According to this model, during irradiation, a part of the electrons freed by the ionizing radiation are captured by traps. Later, when the sample is heated, the trapped electrons jump into the conduction band,

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from where they might either recombine with a hole in the recombination center, or might be recaptured by the trap. The recombination of electrons gives rise to the emission of light. Unfortunately, from the set of differential equations describing the carrier traffic among traps, recombination centers and energy bands it is not possible to obtained a closed expression for $I_{th}(T,\alpha)$. An analytical expression for the emitted light is necessary because the set of parameters is usually found by fitting the theoretical expression $I_{th}(T,\alpha)$ to the recorded light $I_{exp}(T)$. Frequently the fitting is accomplished by resorting to algorithms, such as the Levenberg-Marquardt algorithm (L-M) [1].

In order to obtain an analytical expression an approximation is made, dubbed quasi-equilibrium approximation (QE). The QE approximation assumes that $\frac{dn_c}{dt} \cong 0$ and $n_c \ll n$. As shown in reference [2], the light intensity is given by:

$$I(T) = \frac{n(T).s\exp\left(-\frac{E}{kT}\right)h(T)A_m}{\left(N - n(T)\right)A_n + hA_m} \tag{1}$$

where A_n and A_m stand for the retrapping and the recombination cross section respectively. A kinetics, known as first order kinetics (FO), results if it is further assumed that retrapping is negligible against recombination, i. e., $\left(N - n(T)\right)A_n \ll hA_m$ [2]:

$$I(T) = n(T).s\exp\left(-\frac{E}{kT}\right) \tag{2}$$

Since the QE approximation entails that $n_c(T) \approx 0$ from charge neutrality it results m(T)=n(T). Taking into account that

$I(T) = -\frac{dm(T)}{dT} = -\frac{dn(T)}{dT}$, this equation along with equation 2 yield:

$$I(T) = n_0.s\exp\left(-\frac{E}{kT}\right)\exp\left(-\frac{s}{\beta}\int_{T0}^{T}\exp\left(\frac{E}{ku}\right)du\right) \tag{3}$$

On the contrary, if retrapping prevails on recombination, i. e., $\left(N - n(T)\right)A_n \gg hA_m$, the following equation results:

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$$I(T) = s.\left(\frac{A_n}{NA_m}\right).n^2\, exp\left(\frac{-E}{kT}\right) \quad (4)$$

From this equation one can obtain:

$$I(T) = n_0^{\,2} s' exp\left(\frac{-E}{kT}\right)\left[1+\frac{n0s'}{\beta}\int_{T0}^{T} exp(-\frac{E}{ku})du\right]^{-2} \quad (5)$$

In Eq. 5 s' stands for $\frac{s.A_n}{NA_m}$. Garlick and Gibson put forward this kinetics, called second order kinetics (SO) [3].

Since a closed expression cannot be derived when recombination does not prevail on retrapping, or retrapping on recombination, May and Partridge put forward a heuristic expression with the aim of describing kinetics comprised between first and second order [4]:

$$I(T) = n_0.s'' exp(-\frac{E}{kT})\left[1+(b-1)\frac{s''}{\beta}\int_{T0}^{T} exp(-\frac{E}{ku})du\right]^{\frac{-b}{b-1}} \quad (6)$$

In this equation s'' stands for $s'.n_0^{\,b-1}$, and β for heating rate. b is a parameter loosely related to the retrapping probability. When b→1 Eq. 6 converges to FO kinetics, and when b=2, to SO kinetics. This kinetics is known as the general order kinetics (GO), and it is nowadays the most employed kinetics for analyzing glow curves.

Several authors have investigated the validity of the GO kinetics. According to the reported results the GO kinetics suffers from several flaws:

1) Investigations have been carried out to find a connection between b and physically meaningful models, but a clear relationship could not be established [5, 6]
2) Moharil and Opanowicz found that the kinetic order b is usually not constant during thermal stimulation and should not be used for characterization of thermoluminescence [7, 8].
3) It has been reported that the GO model has limitations for determination of the activation energy [9].

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4) By resorting to computer simulation Sakurai has shown that the GO kinetics yields wrong parameters [10]. Furthermore, he states that one of the defects of the GO kinetics arises from the fact that traffic of electrons (or holes) among traps is ignored [11].
5) Basun et al. have shown that the interaction among traps affects the shape of glow curves, thus affecting the parameters given by the GO kinetics [12].
6) There is a difficulty with Eq. 6, namely, the dimension of the pre-exponential factor s'' has an unacceptable meaning because it varies in the same sample when the dose is changed. In order to overcome this problem Rasheedy put forward a modified expression [13].

$$I(T) = \frac{n_0^{\,b}}{N^{b-1}}.s\exp(-\frac{E}{kT})\left[1+(b-1)\frac{s.n_0^{\,b-1}}{\beta.N^{b-1}}\int_{T0}^{T}\exp(-\frac{E}{ku})du\right]^{\frac{-b}{b-1}} \quad (7)$$

This equation can be written:

$$I(T) = N.x_0^{\,b}.s\exp(-\frac{E}{kT})\left[1+(b-1)\frac{s.x^{b-1}}{\beta}\int_{T0}^{T}\exp(-\frac{E}{ku})du\right]^{\frac{-b}{b-1}} \quad (8)$$

In Eq. 8 x stands for n/N, namely, x is the filling factor of the trap, and x_0 is the filling factor before the recording of the glow curve. Since x has no dimension, the dimension of s does not depend on dose ($Dose \prec x_0$).

In spite of the aforementioned drawbacks, nowadays the original GO kinetics given by Eq. 6 is the most employed kinetics for analyzing glow curves. To the best of our knowledge no investigations has been carried out on the validity of the GO kinetics put forward by Rasheedy.

The aim of the investigation reported in this article was twofold: 1) to evaluate the validity of the new GO kinetics, and how the parameters compare to the parameters obtained with the old version, and 2) to find a criterion to assess whether the parameter found with the GO kinetics are accurate or acceptable estimates of the true parameters. To this end

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synthetic glow curves were generated for the model shown in figure 1, which were analyzed with both versions of the GO kinetics.

Differential equations

For the OTOR model the set of differential equations describing the carrier traffic are:

$$\frac{dn}{dT} = -\frac{s}{\beta}.n\,exp(-\frac{E}{kT}) + \frac{A_n}{\beta}\left[N-n\right]n_c \qquad (9)$$

$$\frac{dh}{dT} = -\frac{A_m}{\beta}n_c.h \qquad (10)$$

$$h = n + n_c \qquad (11)$$

$$I = A_m n_c.h \qquad (12)$$

Taking into account that n(T)=N x(T) the equations read:

$$\frac{dx}{dT} = -\frac{s}{\beta}.x\,exp(-\frac{E}{kT}) + \frac{AN}{\beta}(1-x)n_c'$$

$$\frac{dh'}{dT} = -\frac{AM}{\beta}n'_c.h'$$

$$h' = x + n_c'$$

$$I = N.AM.n_c'.h'$$

h'(T) stands for h(T)/N, n_c'(T) for n_c(T)/N, AN for A_n.N, and AM for A_m.N.

Written in this way the set of differential equations represents different cases having the same AN and AM. For instance, AN=40 1/s and AM= 50 1/s might correspond to the following cases: $A_n = 4{\cdot}10^{-9}$ cm^3/s, $A_m = 5{\cdot}10^{-9}$ cm^3/s, and N= 10^{10} 1/cm^3, or might correspond to $A_n = 4{\cdot}10^{-8}$ cm^3/s, $A_m = 5{\cdot}10^{-8}$ cm^3/s, and N= 10^{11} 1/cm^3. Glow curves were computed for E= 1.04 eV, s= 10^{12} 1/s, and for different values of xo, AN, AM, and heating rates.

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Analysis of glow curves with both GO kinetics.

Instead of Eq. 6 the expression derived by Kitis et al. is employed in most articles [14]:

$$I(T) = \frac{I_M .b^{\frac{b}{b-1}} exp\left[\frac{E}{kT}\left(\frac{T-T_M}{T_M}\right)\right]}{\left[(b-1).(1-\Delta).\frac{T^2}{T_M{}^2} exp\left[\frac{E}{kT}\left(\frac{T-T_M}{T_M}\right)\right] + Z_m\right]^{\frac{b}{b-1}}} \qquad (13)$$

Where

$$s = \frac{\beta.E}{k.T_M{}^2}.\frac{1}{Zm} exp\left(\frac{E}{k.T_M{}^2}\right)$$

$$\Delta = \frac{2k.T}{E} \quad ; \quad \Delta_M = \frac{2k.T_M}{E}$$

$$Z_M = 1+(b-1)\frac{2k.T_M}{E} = 1+(b-1)\Delta_M$$

In the equations above both I_M and T_M stand for the highest intensity of the peak and the corresponding temperature respectively.

Taking into account that capture cross sections vary between 10^{-12} (coulombic attractive center) and 10^{-19} cm^2 (neutral center) [15], and that the thermal velocity of electrons is nearly 10^7 cm/s, A_n and A_m may have values between 10^{-12} and 10^{-5} cm^3/s. Thus for $N \geq 10^{10}$ cm^{-3}, the values of both AN and AM should be higher than 10^{-2} 1/s. Glow curves were generated with values of AM and AN comprised between 4 and 4000, and for x0=0.01

Defining R=AN/AM, glow curves were computed for R= 0.25, 1.0, and 4.0, and different values of AM. Computed parameters obtained by fitting the synthetic glow curves with both GO kinetics are shown in tables 1, 2 and 3.

Table 1: Computed parameters employing the two versions of the GO kinetics. The synthetic glow curves were calculated for R= 0.25, x0= 0.01 and the AM values indicated in the table.

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	May and Partridge				Rasheedy			
AM (1/s)	E (eV)	s (1/s)	b	FOM (%)	E (eV)	s (1/s)	b	FOM (%)
4	0.67	$1.8\ 10^{6}$	1.0	20.0	1.01	$5.2\ 10^{13}$	3.5	6.4
40	0.97	$7.2\ 10^{9}$	1.1	9.1	1.01	$2.1\ 10^{12}$	2.0	4.2
400	1.05	$5.3\ 10^{10}$	1.5	8.7	1.02	$1.4\ 10^{12}$	1.9	1.9
4000	1.05	$5.7\ 10^{10}$	1.5	9.1	1.02	$1.3\ 10^{12}$	1.9	1.4

Table 2: Computed parameters employing the two versions of the GO kinetics. The synthetic glow curves were calculated for R= 1.0, x0=0.01 and the AM values indicated in the table.

	May and Partridge				Rasheedy			
AM (1/s)	E (eV)	s (1/s)	b	FOM (%)	E (eV)	s (1/s)	b	FOM (%)
4	0.67	$9.4\ 10^{5}$	1.0	18.5	0.96	$6.9\ 10^{12}$	3.1	6.7
40	0.97	$2.0\ 10^{9}$	1.4	6.0	1.03	$1.4\ 10^{12}$	2.1	2.7
400	1.04	$1.6\ 10^{10}$	1.5	9.3	1.04	$1.0\ 10^{12}$	2.0	0.8
4000	1.04	$1.1\ 10^{10}$	1.5	9.8	1.04	$1.0\ 10^{12}$	2.0	0.3

Table 3: Computed parameters employing the two versions of the GO kinetics. The synthetic glow curves were calculated for R= 4, x0= 0.01 and the AM values indicated in the table.

	May and Partridge				Rasheedy			
AM (1/s)	E (eV)	s (1/s)	b	FOM (%)	E (eV)	s (1/s)	b	FOM (%)
1	0.59	$4.2\ 10^{4}$	1.0	31.0	0.81	$1.7\ 10^{13}$	4.7	6.0
10	0.80	$2.9\ 10^{8}$	1.1	14.3	1.03	$1.8\ 10^{12}$	2.5	4.0
100	1.03	$2.0\ 10^{9}$	1.5	9.0	1.06	$8.6\ 10^{11}$	2.1	1.1
1000	1.05	$3.4\ 10^{9}$	1.5	9.0	1.06	$6.4\ 10^{11}$	2.0	0.8

From the tables the following remarks can be done: 1) the parameters obtained with the original GO kinetics differ significantly from the true values for the two lowest values of AM, while for new version only for the lowest AM, 2) for the three highest values of AM the original GO kinetics gives frequency factors that differ at least three order of magnitude from the true value, while for the new version the differences are less than one order of magnitude, and 3) the energies given by the new version for the three highest values of AM

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differ from the true values by less than 2%, while for the original version only for the two highest values of AM.

It follows from the remarks above that the new version of the GO kinetics yield more reliable frequency factors than the original version, and activation energies for a larger interval of AM's. Mady et al. reported that one factor that controls the thermoluminescence response is x0 [16]. This factor is taken into account in the new version of the GO kinetics.

Figure 2 shows concentration of trapped electrons and the concentration of electrons in the conduction band for R=1 and AM= 4, 40 and 400. For AM= 4000 no figure is shown because the concentration of electrons in the conduction band is negligible against the concentration of trapped electrons. Similar results are obtained for R= 0.25 and R= 4.

Comparing the results shown in the tables and in the figures it can be concluded that the difference between the parameters given by both GO kinetics and the true values increases as the normalized concentration of electrons n_c/n_0 in the conduction band increases. For a negligible concentration of electrons in the conduction band the new version of the GO kinetics yields good estimates of the activation energy and frequency factors.

Fig. 2: Normalized concentration of trapped electrons n/n0 (solid line) and electrons in the conduction band n_c/n_0 (dash line) for (a) AM= 4 and R= 1, (b) for AM= 40 and R= 1 and (c) for AM= 400 and R= 1.

From tables 1-3 and figure 2 can be concluded that the computed parameters worsen as the relationship n_c/n_0 increases.

For a given material irradiated with a given dose the concentration of electrons n_c will increase as the heating rate increases because more electrons will be injected into the conduction band in a given time interval, as it is illustrated in figure 3.

Fig. 3: Concentration n of trapped electrons and concentration n_c of electrons in the conduction band, both normalized to the initial concentration n_0 of trapped electrons. A: heating rate of 1 K/s. B: heating rate of 5 K/s.

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If n_c/n_0 is negligible for a given heating rate, say 1K/s, and n_c/n_0 remains negligible for higher heating rates, say 3 and 5 K/s, the computed trap parameters should not change or change little. To verify whether this assumption is correct, synthetic glow curves for heating rates of 1, 3 and 5 K/s were computed and analyzed with the new version of the GO kinetics for the case R=1 shown in table 4. Similar results are obtained for R= 0.25 and R= 4.

Based on the data shown in table 4, the following conclusions can be drawn:

1) As expected, the computed parameters change as the heating rate increases.
2) Computed parameters close to the true ones are obtained when the parameters change little by increasing the heating rate. In these cases the FOM's are lower than 5%.
3) If the computed parameters change little with heating rates, then the parameters obtained with the lowest heating rate can be considered a good estimate of the parameters.

The results reported so far were computed for x0= 0.01, namely, for a low dose. Recently Sadek et al. reported that the original GO kinetics fails for a saturated trap if $A_n > A_m$ [17]. Glow curves were computed for the parameters employed above, except that x_0 was given the value of 1, namely, the trap is saturated. Table 5 shows the computed parameters for $x_0 = 1$ by employing both the original and new version of the GO kinetics.

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Table 4: Computed parameters for three heating rates. R=1 and x0=0.01

AM (1/s)	Parameters	1 K/s	3 K/s	5 K/s
	E (eV)	0.96	0.87	0.80
	s (1/s)	$6.9\ 10^{12}$	$1.0\ 10^{13}$	$1.1\ 10^{13}$
4	b	3.1	4.4	5.1
	x0	0.020	0.028	0.030
	FOM (%)	6.7	6.0	6.0
	E (eV)	1.03	1.03	1.02
	s (1/s)	$1.4\ 10^{12}$	$1.6\ 10^{12}$	$1.8\ 10^{12}$
40	b	2.1	2.4	2.6
	x0	0.011	0.012	0.013

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	FOM (%)	2.7	4.9	3.8
	E (eV)	1.04	1.05	1.06
	s (1/s)	$1.0\ 10^{12}$	$7.7\ 10^{11}$	$7.5\ 10^{11}$
	b	2.0	2.0	2.0
400	x0	0.010	0.009	0.009
	FOM (%)	0.8	0.8	1.1
	E (eV)	1.04	1.06	1.06
	s (1/s)	$1.0\ 10^{12}$	$7.6\ 10^{11}$	$6\ 10^{11}$
4000	b	2.0	2.0	2.0
	x0	0.0100	0.0095	0.0092
	FOM (%)	0.3	0.7	0.9

β=1 K/s

Table 5: For AM= 1000 1/s and R= 4 the computed parameters for three heating rates are shown.

β=1 K/s

	E (eV)	s (1/s)	b	FOM (%)
Kitis	0.76	$1.4\ 10^{8}$	1.4	11.0
Rasheedy	0.86	$3.4\ 10^{9}$	2.2	5.5

β=3 K/s

	E (eV)	s (1/s)	b	FOM (%)
Kitis	0.76	$6.5\ 10^{7}$	1.4	12.2
Rasheedy	0.85	$1.6\ 10^{9}$	2.2	5.4

β=5 K/s

	E (eV)	s (1/s)	b	FOM (%)
Kitis	0.76	$4.4\ 10^{7}$	1.4	12.4
Rasheedy	0.85	$1.1\ 10^{9}$	2.2	5.3

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The results make evident that both versions fail to yield the true parameters. In table 5 the values of x_0 given by the new version are not listed. They are x_0= 0.919 (β= 1 K/s), 0.756 (β= 3 K/s), and 0.60 (β= 5 K/s). These values change significantly with heating rate even though according to the calculations the QE approximation holds.

Table 6: Parameters computed for AM= 4, R= 0.25, and x0= 1, and three different heating rates.

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	β= 1 K/s	β= 3 K/s	β= 5 K/s
E (eV)	1.06	1.08	1.10
s (1/s)	$1.4\ 10^{12}$	$9.1\ 10^{11}$	$9.6\ 10^{11}$
b	1.4	1.5	1.6
x0	0.965	0.824	0.767
FOM (%)	3.8	5.1	5.6

Table 7: Parameters computed for AM= 4000, R= 0.25 and x_0= 1, and three different heating rates

	β= 1 K/s	β= 3 K/s	β= 5 K/s
E (eV)	1.05	1.08	1.10
s (1/s)	$1.4\ 10^{12}$	$1.2\ 10^{12}$	$1.0\ 10^{12}$
b	1.4	1.5	1.5
x0	0.965	0.977	0.988
FOM (%)	3.8	3.1	3.8

Tables 6 and 7 show the parameters obtained for x_0 = 1, R= 0.25, and AM= 4 and 4000. For this case (R<1), the values do not change significantly, and the values for β= 1 K/s are close to the true ones, namely, they are good estimates of the parameters.

An important issue, not reported so far to the best of our knowledge, is how to assess the accuracy of the parameters obtained by deconvolving an experimental glow curve with the GO kinetics. A clue to find a criterion is given by the results reported so far: if the values of the computed parameters change little for different heating rates, then the values for β =1K/s are close to the values employed for generating the synthetic glow curves. For example, for AM= 4000 in table 4, for β= 1, 3 and 5 K/s the values E varies between 1.04 and 1.06 eV, the values of s between $6\ 10^{11}$ and $1\ 10^{12}$ 1/s, and the values of x_0 between 0.0092 and 0.0100, and b does not change. The parameters for β= 1K/s coincide with the true ones. In table 5 the parameters E, s and b change little, but x0 varies between 0.06 and 0.89, thus the values for β= 1 K/s differ from the correct values.

So far the reported results correspond to a model with one trap. Most of the thermoluminescence materials show two or more traps. As reported above, the interaction among traps affects the shape of the glow curve, and consequently the GO kinetics yield incorrect parameters. As shown in reference [18], electrons released by a trap might be captured by another trap. Thus a peak might not be related to the electrons occupying a

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specific trap before the recording of a glow curve, as it is assumed in the GO kinetics. This fact has been also pointed out in a recent article [19]. One can expect that the GO kinetics will give acceptable estimates of the parameters if the capture of electrons by traps is negligible, namely, the second term on the right side of Eq. 9 is negligible. Then the set equation related to two traps, each one indicated with the subscript i is:

$$\frac{dn_i(T)}{dT} = -\frac{s_i}{\beta} n_i(T) exp(-\frac{E_i}{kT}) \qquad \text{i=1, 2} \qquad (14)$$

$$\frac{dh(T)}{dT} = -\frac{AM}{\beta} n_c(T).h(T) \qquad (15)$$

$$h(T) = n_1(T) + n_2(T) + n_c(T) \qquad (16)$$

$$I(T) = AM.n_c(T).h(T) \qquad (17)$$

A particular case of non-interacting traps is the first order kinetics, which is derived from the set of differential equations 14-17 by assuming another approximation, i. e., the quasi-equilibrium approximation.

The set of equations has been solved for the following values of parameters: $s_1=s_2=10^{12}$ s^{-1}, $n_{01} = n_{02} = 10^{10}$ cm^{-3}, $E_1 = 1.04$ eV, $E_2 = 1.17$ eV, and three values of A_m, namely, $4 \cdot 10^{-7}$, $8 \cdot 10^{-8}$ and $4 \cdot 10^{-11}$ cm^3/s. The results are listed in table 8.

Table 8: Parameters computed with the new version of the GO kinetics.

A_m (cm^3/s)	s_1 (1/s)	E_1 (eV)	b_1	s_2 (1/s)	E_2 (eV)	b_2
$4\ 10^{-7}$	$1.07\ 10^{12}$	1.04	1.01	$1.08\ 10^{12}$	1.17	1.01
$4\ 10^{-8}$	$1.07\ 10^{12}$	1.04	1.01	$1.05\ 10^{12}$	1.16	1.07
$4\ 10^{-11}$	$9.11\ 10^{11}$	1.03	1.03	$1.8\ 10^{12}$	1.13	1.40

For $A_m = 4 \cdot 10^{-7}$ cm^3/s the values of the parameters coincide with the true values. The values of b for both traps are close to 1, which indicates FO kinetics. For $A_m = 4 \cdot 10^{-11}$ cm^3/s the energy E_1 differs from the true value by less than 1%, and the energy E_2 by less than 3.5 %. Thus for $A_m = 4 \cdot 10^{-11}$ cm^3/s the computed parameters are acceptable estimates. In this case

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FO kinetics is not valid because the quasi-equilibrium approximation does not hold, as shown in figure 4. This is the reason why b2 is higher than 1 (accumulation of electrons in the conduction band brings about a widening of peaks, which in turn leads to values of b higher than 1).

For $A_m = 4 \cdot 10^{-8}$ cm^3/s the parameters are excellent estimates of the true values. This is an intermediate case between $A_m = 4 \cdot 10^{-7}$ cm^3/s and $A_m = 4 \cdot 10^{-11}$ cm^3/s.

Figure 4: Concentration of trapped electrons (solid line), and concentration of electrons in the conduction band (dash line).

Thus for TL-materials having two or more traps the following criteria is put forward:

1) Glow curves for different doses should be recorded. If the glow curve does not shift to lower temperatures as the dose increases the interaction among peaks may be ignore. The shape of the glow curve might vary because of the different concentration of traps and their recombination probabilities.
2) For a low dose glow curves for three different heating rates should be recorded employing the new version of the GO kinetics. If the parameters E, s, x0, and b change little, say by less than 4% , and the frequency factors differ by less than one order of magnitude, the parameters for β=1 K/s are acceptable estimates.

In the next section the analysis of three glow curves corresponding to three heating rates of the compound YVO_4: Eu^3 is reported. This compound was chosen because it has a high radioluminescence, which entails a high recombination probability. Thus we expect that interaction among traps will not affect significantly the glow curves, and consequently, the new version of the GO kinetics will yield acceptable parameters.

Trap parameters of YVO_4: Eu^{3+} compounds.

Glow curves recorded with a heating rate of 1 K/s could not be fitted with a model of two traps. Therefore a model with three traps was considered for the analysis of glow curves.

Glow curves of the YVO_4: Eu^{3+} compounds were recorded for three different heating rates, namely 1, 3 and 5 K/s. Glow curves recorded for different doses do not shift to lower temperatures, so that the GO kinetics may be used. The parameters computed by analyzing

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the three glow curves are shown in table 9. They were computed by employing the Levenberg-Marquardt algorithm [1]. The glow curves and the curves found from the fitting procedure are shown in figure 5.

Table 9: Computed parameters from three glow curves of YVO_4: Eu^{3+}, recorded for three different heating rates.

β (K/s)	s1 (1/s)	E1 (eV)	b1	x01	s2 (1/s)	E2 (eV)	b2	x02	s3 (1/s)	E3 (eV)	b3	x03	FOM (%)
1	$2.5\ 10^{12}$	0.85	1.8	0.018	$1.2\ 10^{12}$	1.05	1.0	0.0027	$2.7\ 10^{12}$	1.15	1.3	0.0097	3.6
3	$3.1\ 10^{12}$	0.85	1.8	0.017	$1.2\ 10^{12}$	1.07	1.0	0.0027	$3.9\ 10^{12}$	1.16	1.3	0.0097	4.3
5	$2.5\ 10^{12}$	0.85	1.8	0.017	$1.9\ 10^{12}$	1.07	1.0	0.0029	$3.9\ 10^{12}$	1.15	1.3	0.0093	4.5

Figure 5: Recorded (open circle) and fitted (solid line) glow curves recorded (a) with β= 1K/s , (b) with β= 3K/s, and (c) with β= 5 K/s

The parameters listed in table 9 change little with the heating rate. Thus according to the criterion put forward before the computed parameters for β=1 K/s are accurate or acceptable estimates of the true parameters.

Conclusions

According to the reported results the following conclusions can be drawn:

1) The new version of the GO kinetics gives more acceptable parameters for a wider range of recombination and retrapping probabilities than the original version.
2) The original version yields always frequency factors, which differs significantly from the correct ones.

Therefore the new version of the GO kinetics should be employed for analyzing glow curves.

In the case of two or more traps the new GO kinetics can be employed if the retrapping of every trap is negligible. This can be verified by recording glow curves for different doses and observe whether the position of the peaks shift to lower temperatures as the dose increases. If no significant shift is observed, then the new version of the GO kinetics may be employed.

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Finally the criterion based on the recording of glow curves for three different heating rates should be employed to assess the accuracy of the computed parameter: the doses given to a sample must be low, and if the parameters computed for different heating rates change little, then the parameters obtained with the lowest heating rate β are accurate or acceptable estimates of the true ones.

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Fig. 1

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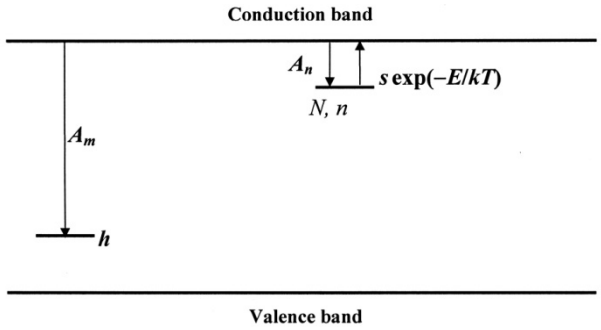

Fig. 2

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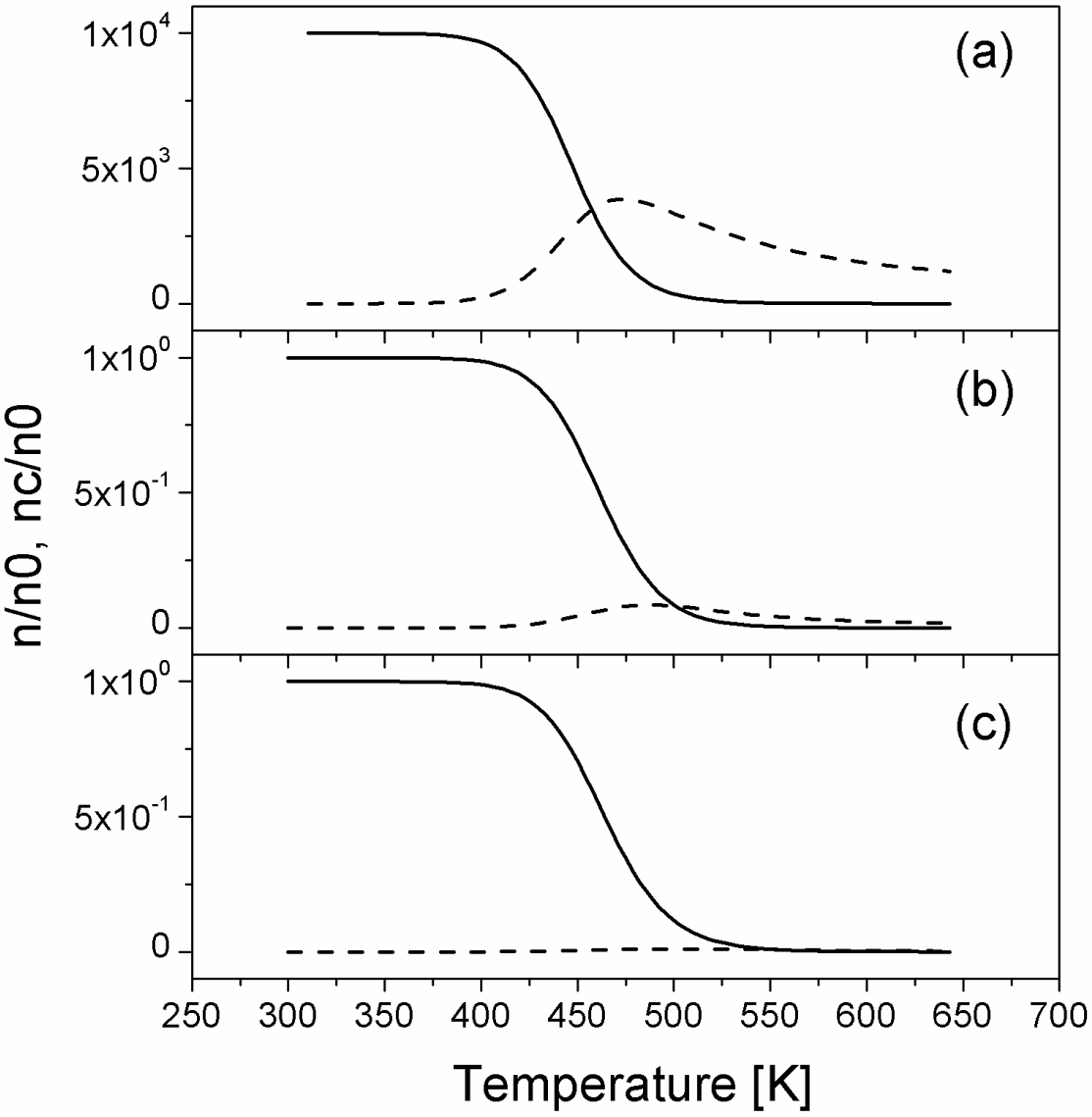
1x10^4
5x10^3
0
(a)
1x10^0
5x10^-1
0
(b)
1x10^0
5x10^-1
0
(c)
n/n0, nc/n0
250
300
350
400
450
500
550
600
650
700
Temperature [K]

Fig. 3

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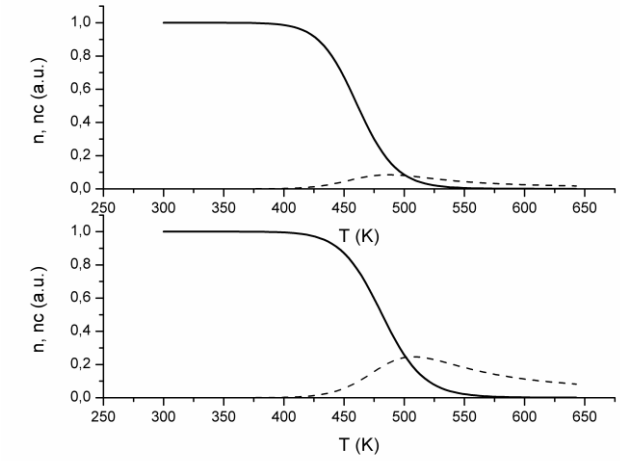


Fig. 4

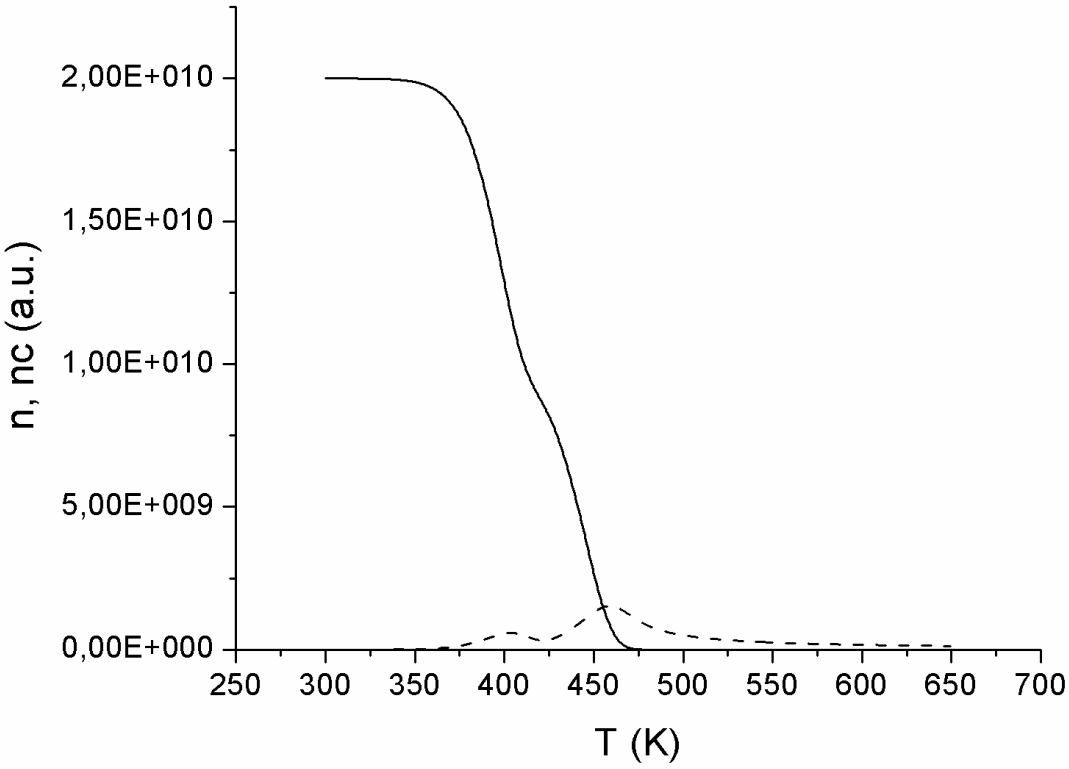
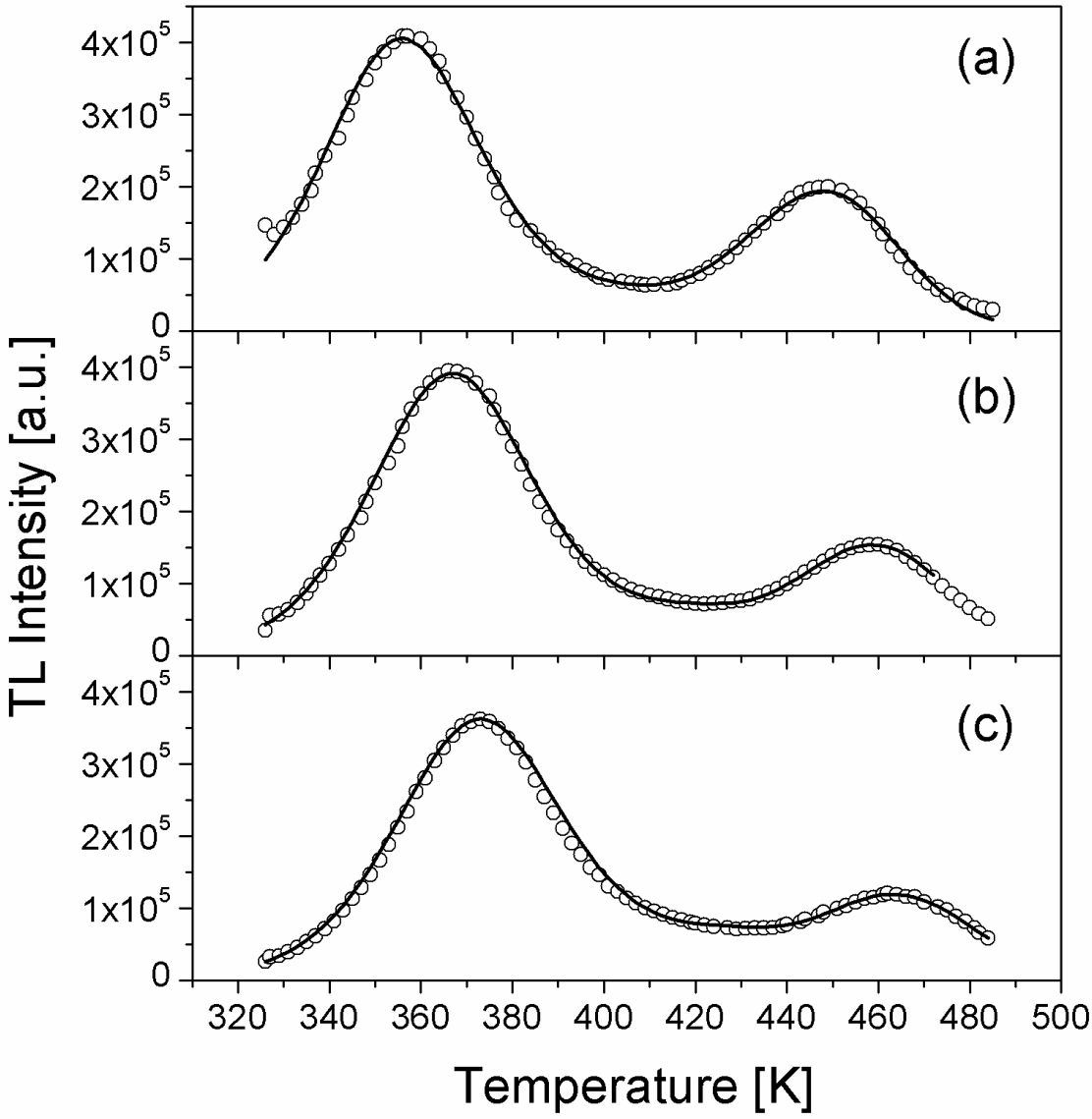


Fig. 5

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