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A new method for obtaining the order of kinetics and the activation energy of the thermoluminescence glow peak

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Abstract. The order of kinetics b of the thermoluminescence (TL) glow peak is usually determined once its symmetry factor μ_g is known. In the present work, an equation is suggested to estimate directly the order of kinetics b of the glow peak. The value of b can be obtained by using the values of the temperatures T_m (K), T_1 (K) and T_2 (K) at the maximum intensity and half maximum intensities of the peaks, respectively and the peak areas A_m , A_1 and A_2 estimated from T_m , T_1 and T_2 to the final temperature of the glow peak, respectively. Also, the activation energy E (eV) can be obtained after evaluating the order of kinetics b. The methods were checked for numerically computed TL glow peaks. The results are in good agreement with the given values of the order of kinetics b and activation energy E.

1. Introduction

Thermoluminescence (TL) is the thermally stimulated light emitted from an insulator or semiconductor when it is heated as a result of previous exposure to ionizing radiation. Experimental results are usually presented as a light intensity as a function of temperature or time. The resulting curve of intensity against temperature, or time, is called a glow curve and contains one or more glow peaks. The glow peaks are analysed usually by assuming first- [1], second- [2] and general- [3,4] order kinetics. The shape, position and intensity of the TL glow peaks are related to various trapping parameters of the trapping states responsible for the TL emission. These parameters include the frequency factor S (s⁻¹), the activation energy E (eV) and the order of kinetics b. For a characterization of the single TL peak Halperin and Braner [5] introduced a parameter called the symmetry factor (see figure 1):

$$\mu_g = \frac{T_2 - T_m}{T_2 - T_1} \tag{1}$$

where T_m (K) is the temperature corresponding to the maximum of TL intensity, I_m , of the glow peak; T_1 (K) and T_2 (K) are the temperatures at which the TL intensity is equal to half of the maximum intensity on either side of T_m ($T_2 > T_1$).

A number of research workers [6–18] have used the symmetry factor μ_g to determine the order of kinetics of TL glow peaks in various materials. Also, the determination of the order of kinetics from the symmetry factor has been the topic of discussion in several papers [14,19–24]. Moreover, other forms of the symmetry factor rather than the form appearing in equation (1) are obtained and a discussion of their validities for the determination of the order of kinetics has been given by several authors [14,25,26]. For example, Balarin [25] has suggested checking $(T_2 - T_m)/(T_m - T_1)$ which should be 0.7 to 0.8 for first-order

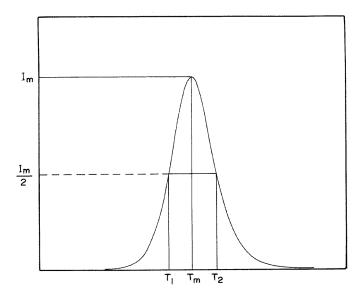


Figure 1. An isolated glow peak showing the glow curve shape parameters.

and 1.05 to 1.2 for second-order kinetics. Also, Gartia *et al* [14] have pointed out that the symmetry factor should be checked not only at a point where the intensity is equal to one-half, but at any other suitable point selected in [14] such as two-thirds or four-fifths of the intensity. Gartia and Singh [26] have studied the change of μ_g with n_0/N , where n_0 (cm⁻³) is the concentration of trapped carriers at the beginning of the read-out, and N (cm⁻³) is the concentration of traps. They have found that the value of the symmetry factor μ_g of the second-order glow peaks is not independent of the ratio n_0/N .

In the present work, an expression is suggested in which it becomes possible to estimate easily the kinetics order b of the TL glow peak. Also, the value of the activation energy (E) can be obtained after evaluating the order of kinetics b.

2. Theoretical background

2.1. First-order kinetics

The first theoretical treatment for a well isolated TL peak was given by Randall and Wilkins, who mainly considered the non-retrapping case and assumed a TL intensity proportional to the concentration of trapped electrons [1]. This case is usually called first-order kinetics. The rate of release of electrons per unit time (s) at a temperature T (K) is given by

$$I = -\frac{\mathrm{d}n}{\mathrm{d}t} = nS \exp(-E/kT) \tag{2}$$

where I (in arbitrary units) is the TL intensity, n (cm⁻³) the electron concentration trapped at time t (s) and k (eV K⁻¹) the Boltzmann constant. The equation describing TL intensity for first-order kinetics is then given by [1]

$$I = n_0 S \exp(-E/kT) \exp\left[-\frac{S}{R} \int_{T_0}^T \exp(-E/kT') dT'\right]$$
 (3)

where R (K s⁻¹) = dT/dt is the linear heating rate and n_0 (cm⁻³) is the concentration of traps populated at the starting temperature T_0 (K).

2.2. Second-order kinetics

Taking into account the retrapping process, Garlick and Gibson assumed that the TL intensity is proportional to the squared concentration of trapped electrons [2]. This case is referred to as second-order kinetics. The rate of release of electrons per unit time at a temperature T (K) is given by [2]

$$I = -\frac{\mathrm{d}n}{\mathrm{d}t} = \frac{n^2 S}{N} \exp(-E/kT) \tag{4}$$

where N (cm⁻³) is the concentration of traps. The equation describing TL for second-order kinetics according to equation (4) is given by [2]

$$I = \frac{n_0^2 S \exp(-E/kT)}{N \left[1 + \left[\frac{n_0 S}{NR}\right] \int_{T_0}^T \exp(-E/kT') dT'\right]^2}.$$
 (5)

2.3. General-order kinetics

The first- and second-order equations for TL are special cases of a more general equation given by Halperin and Braner [5]. May and Partridge [27,28] and others [3,29–33] have proposed the following empirical equation when neither conditions for first order nor those for second order are satisfied:

$$I = -\frac{\mathrm{d}n}{\mathrm{d}t} = n^b S' \exp(-E/kT) \tag{6}$$

where b is the order of kinetics and S' (cm^{3(b-1)} s⁻¹) the pre-exponential factor. Usually b is assumed to be between one and two, but sometimes it can exceed this range [3]. The solution of equation (6) for a linear heating rate R and for $b \neq 1$ is given by [3]

$$I = \frac{n_0 S \exp(-E/kT)}{\left[1 + \frac{(b-1)S}{R} \int_{T_0}^T \exp(-E/kT') dT'\right]^{b/(b-1)}}$$
(7)

where S, defined by Chen [34], has the units of s^{-1}

$$S = S' n_0^{(b-1)}. (8)$$

Recently, and for some difficulties related to the dimensions in equations (6) and (8), we have presented a modification of the general-order equation as [4]

$$I = -\frac{\mathrm{d}n}{\mathrm{d}t} = \frac{n^b}{N^{b-1}} S \exp(-E/kT) \tag{9}$$

which includes the better known first- and second-order cases given in equations (2) and (4), respectively. The solution of equation (9) for a linear heating rate R and for $b \neq 1$ is given by [4]

$$I = \frac{n_0^b N^{1-b} S \exp(-E/kT)}{\left[1 + \left[\frac{S(b-1)(n_0/N)^{(b-1)}}{R} \int_{T_0}^T \exp(-E/kT') dT'\right]\right]^{b/(b-1)}}.$$
 (10)

3. The basis of the present work

We now present the mathematical details of the present work based on which it is possible to calculate the area of a part from the glow curve at certain temperature. Following Moharil [35–38], it is assumed that the glow curve consists of a single glow peak, corresponding to traps of only one kind. It is also assumed that at the end of the glow curve all the traps are emptied. Then, the concentration of traps populated at the beginning of the glow curve, n_0 , is proportional to the area under the glow curve. Again, the concentration of traps emptied up to the temperature T_i is given by the area under the glow curve up to T_i . Hence, the concentration of populated traps at temperature T_i during the TL run is proportional to the area A_i which is equal to the total area under the glow curve less the area under the glow curve between the initial point and T_i . Thus, A_i is equal to the area under the glow curve between the T_i and T_f , where T_f is the temperature at which the TL intensity falls to zero after reaching a maximum value as shown in figure 2. Now, consider the maximum intensity of the glow peak, I_m ; equation (6) thus becomes

$$I_m = (A_m)^b S' \exp(-E/kT_m) \tag{11}$$

where A_m is the area under the glow curve between T_m and T_f . In analogue to equation (11), using equation (9) one obtains

$$I_m = \frac{(A_m)^b}{N^{b-1}} S \exp(-E/kT_m).$$
 (12)

Now, assuming that $I_1 = (I_m/2)$ and $I_2 = (I_m/2)$ are the half-maximum intensities, and these occur at temperatures T_1 (K) and T_2 (K), respectively, then, similar to equation (12), the following equations may be written:

$$I_1 = I_m/2 = \frac{(A_1)^b}{N^{b-1}} S \exp(-E/kT_1)$$
 (13)

$$I_2 = I_m/2 = \frac{(A_2)^b}{N^{b-1}} S \exp(-E/kT_2)$$
 (14)

where A_1 and A_2 indicate the areas under the glow curve from temperatures T_1 to T_f , and T_2 to T_f , respectively, in which T_f is the final temperature of the glow peak.

From equations (12) and (13) one obtains

$$\ln(2) = b \ln\left[\frac{A_m}{A_1}\right] - \frac{E}{k} \left[\frac{1}{T_m} - \frac{1}{T_1}\right] \tag{15}$$

and from equations (12) and (14) one obtains

$$\ln(2) = b \ln \left[\frac{A_m}{A_2} \right] - \frac{E}{k} \left[\frac{1}{T_m} - \frac{1}{T_2} \right]. \tag{16}$$

Equation (15) can be rewritten as

$$E = \left[\ln 2 - b \ln \left[\frac{A_m}{A_1}\right]\right] \left[\frac{kT_m T_1}{T_m - T_1}\right]. \tag{17}$$

Also, equation (16) can be rewritten as

$$E = \left[\ln 2 - b \ln \left[\frac{A_m}{A_2}\right]\right] \left[\frac{kT_m T_2}{T_m - T_2}\right]. \tag{18}$$

Now, equating equations (17) and (18) one can easily obtain

$$b = \frac{T_m[T_1 - T_2] \ln(2)}{T_1[T_m - T_2] \ln\left[\frac{A_m}{A_1}\right] - T_2[T_m - T_1] \ln\left[\frac{A_m}{A_2}\right]}.$$
 (19)

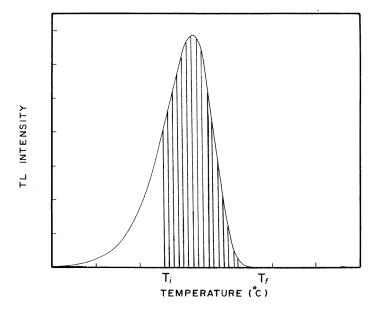


Figure 2. An isolated TL glow peak. The shaded area between T_i and T_f is A_i as defined in the text.

Now, the order of kinetics b can be obtained after evaluating the values of the parameters involved in equation (19). Also, the activation energy E can be obtained after evaluating the order of kinetics b by using equation (17) or (18).

4. Results and discussion

Earlier authors have suggested several analytical methods to obtain the kinetics order of an isolated TL glow peak which cannot be explained by the usual first- or second-order kinetics. The most important method for obtaining the order of kinetics b is the use of the symmetry factor μ_g described in equation (1). Chen [39] has shown that a first-order peak is characterized by a symmetry factor $\mu_g \simeq 0.42$ and a second-order one by $\mu_g \simeq 0.52$, where μ_g is only slightly dependent on the activation energy E and the frequency factor E. Later, Chen [3] numerically solved equation (7), and calculated the symmetry factor E0 for values of E1 numerically solved equation (7), and calculated the symmetry factor E1 for values of E2 between 0.1 eV and 1.6 eV and in the range of E3 between 10⁵ s⁻¹ and 10¹³ s⁻¹. The resultant variation of E1 with E2 is represented here in figure 3 [3]. In this graph the upper and lower curves give the limits of variation of E3 values when the activation energy E3 and the frequency factor E3 are varied, whereas the centre curve shows the average values. The possible error for a given value of the order of kinetics E3 for extreme values of E3 has been found not to exceed E3. The order of kinetics can thus be estimated by using this graph.

The technique of TL has been widely used by a number of workers as a tool to determine the trapping parameters, namely, the activation energy E, the frequency factor S and the order of kinetics b. Among with the other trapping parameters, the determination of the order of kinetics b has special importance, since most of the experimental methods of obtaining the activation energy E require a priori knowledge of the order of kinetics. These methods include the glow curve shape methods, different heating rate methods and

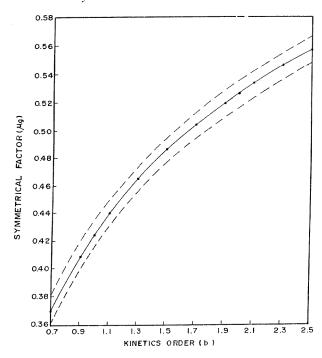


Figure 3. Calculated symmetrical factor μ_g as a function of the given kinetics order b. The solid line is the average value, whilst the dashed lines correspond to the largest possible variation (for various values of E and S). (After Chen [3].)

isothermal decay methods. Detailed explanations of these methods are given in the literature [12, 15, 17, 34, 40–43]. Therefore, a major drawback of these methods to obtain E is that one has to know in advance the order of kinetics involved in the process.

On the other hand, the frequency factor $S(s^{-1})$ in the case of first-order kinetics is given by equating the derivative of equation (3) to zero, thus:

$$S = (RE/kT_m^2) \exp(E/kT_m). \tag{20}$$

Similarly, the frequency factor $S(s^{-1})$ in the case of second order is obtained by equating the derivative of equation (5) to zero, thus:

$$S = \frac{(N/n_0)RE \exp(E/kT_m)}{[2kT_m^2] - E\phi[\exp(E/kT_m)]}$$
(21)

where

$$\phi = \int_{T_0}^{T_m} \exp(-E/kT') \, dT'. \tag{22}$$

Recently [44,45], we have discussed the methods and conditions for obtaining the frequency factor S (s^{-1}) in the case of first- and second-order kinetics and we found that the maximum condition of first-order kinetics obtained by equation (20) is not adequate to determine the frequency factor in the case of second-order kinetics as reported by several authors, which should be determined by using equation (21). Hence, in the absence of *a priori* knowledge of the order of kinetics b the determination of the frequency factor S is not possible.

In spite of the graph depicted in figure 3 having been used by several authors to obtain the order of kinetics, we believe that this graph can give a rough but not exact value of the order of kinetics. Hence, any error in estimating b will be followed by several errors in estimating the other trapping parameters involved, e.g., E and S. On the other hand, values of symmetry factors other than that depicted in figure 3 are given in the literature [16, 46]. For example, Ramana and Sastry [16] have obtained a value of $\mu_g = 0.61$. According to figure 3, this value of μ_g cannot be ascribed to any order of kinetics. Also, it is worth noting that Ramana and Sastry in their paper [16] have used equation (20) to estimate the frequency factor S in spite of using $\mu_g = 0.61$. This may mean that $\mu_g = 0.61$ corresponds to first-order kinetics or it may mean ignorance in the use of the exact equation to determine the frequency factor as we have mentioned [44,45]. Also, several authors have reported values of the symmetry factor μ_g which are not equal or approximately equal to 0.42 and 0.52 for the first and second order, respectively [15, 17]. For example, Azorin et al [17] have reported a second-order glow peak with symmetry factor $\mu_g = 0.54 \pm 0.09$ and reported two first-order glow peaks with symmetry factors $\mu_g = 0.41 \pm 0.09$ and $\mu_g = 0.42 \pm 0.07$. These values of the symmetry factors with their errors exceed the values of the order of kinetics reported in figure 3 in the case of first and second order, respectively. Also, Azorin et al [11] have determined the order of kinetics of the main peak appearing at 190 °C of two materials. According to Azorin et al [11], the symmetry factors of the main peak in both materials are 0.48 ± 0.02 and 0.55 ± 0.02 . These symmetry factors, as reported by these authors, correspond to a kinetic order of 1.63 and 2.31, respectively. As shown in figure 3, there is an inconsistency between the symmetry factors appearing in this paper and the meeting order of kinetics obtained from figure 3. Also, according to Chen [3], figure 3 is calculated for values of the activation energy E ranging from 0.1 to 1.6 eV and for values of S ranging from 10^5 s⁻¹ to 10^{13} s⁻¹. In the literature (see for example [34, 42, 43]), glow peaks are characterized with E and S values higher or lower than the range of E and S mentioned above. These values may not be included in the graph given by Chen [3].

Considering all these aspects of the problem and instead of finding the symmetry factor $\mu_{\rm g}$, equation (19) will be used in the present work, which is easier in use for obtaining the order of kinetics b and equation (17) or (18) will be used thereafter to obtain the activation energy E. To check the present method, generated TL glow peaks are used as the experimental data. Values of b, n_0 (cm⁻³), N (cm⁻³), E (eV), S (s⁻¹) and R (K s⁻¹) are chosen and the corresponding TL intensities I_i (in arbitrary units) are calculated using equations (3), (5) and (10), for the first-, second- and general-order kinetics, respectively, and the values of the peak temperatures T_m (K), T_1 (K), T_2 (K) and the peak areas A_m , A_1 , and A_2 (in arbitrary units) are evaluated. Then, equation (19) is numerically solved for these peak parameters to obtain b. Thereafter, equation (17) or (18) is numerically solved to obtain the activation energy E (eV). The results of these calculations are presented in table 1, where (b1) is the order of kinetics of the generated peak, (b2) the order of kinetics obtained by the present method, E1 (eV) the activation energy of generated peak and E2 (eV) the activation energy obtained by the present method. The other terms n_0 , N, S, R, A_1 , A_m , A_2 , T_1 , T_m and T_2 remain as previously defined. Table 1 includes also the symmetry factor μ_g for the different values of the order of kinetics b.

Close inspection of the results appearing in table 1 show values of $\mu_g \neq 0.42$ for the first order and $\mu_g \neq 0.52$ for the second order (samples (103), (104), (105), (115), (116)). Also, table 1 shows several peaks having different values of the order of kinetics b with the same value of μ_g : samples (115) and (118) and (116) and (117). Therefore, for the same value of the symmetry factor μ_g , a set of kinetics orders may be obtained, which cannot be guessed easily by using figure 3. Therefore, equation (19) gives more accurate information

Table 1. Check of equation (19) for obtaining the order of kinetics and equation (17) or (18) for obtaining the activation energy using generated TL glow peaks, where b1 and E1 (eV) are the order of kinetics and the activation energy of the generated peak, and b2 and E2 (eV) are the order of kinetics and the activation energy obtained by the present method, respectively.

	(101)	(102)	(103)	(104)	(105)	(106)	(107)	(108)	(109)
<i>b</i> 1	0.9	0.9	1.0	1.0	1.0	1.0	1.0	1.0	1.5
$n_0 \text{ (cm}^{-3})$	10^{15}	10^{16}	10^{16}	10^{15}	10^{15}	10^{15}	10^{16}	10^{14}	10^{15}
$N \text{ (cm}^{-3})$	10^{15}	10^{16}	_	_	_	_	_	_	10^{15}
$S(s^{-1})$	10^{13}	10^{5}	10^{4}	100	600	3×10^{4}	3×10^{12}	10^{24}	10^{4}
<i>E</i> 1 (eV)	1.6	0.1	0.5	0.35	0.146	0.13	0.9	1.6	0.1
$R (K s^{-1})$	0.5	0.5	2.0	2.0	0.967	11.67	0.2	2.0	0.5
A_1 (a.u.)	20 089.8	82 296.3	66 811.3	83 470.0	40578.8	195 594.0	64 985.4	80 500.0	86720.1
A_m (a.u.)	9294.07	39 396.6	33 576.0	43 197.6	20 868.4	99 456.7	31 197.4	38 055.4	50 436.7
A_2 (a.u.)	1627.37	7224.94	6921.44	9049.85	4324.91	20 532.1	6036.32	7274.78	14 288.5
T_1 (K)	533.36	75.71	427.91	431.66	157.56	127.36	306.835	321.48	86.16
T_m (K)	555.56	83.06	476.41	503.66	180.36	144.01	320.26	329.72	96.36
T_2 (K)	570.56	88.36	514.16	563.46	198.96	157.31	329.885	335.46	107.01
<i>b</i> 2	0.90078	0.903 64	1.007 66	0.99149	0.997 14	1.00094	1.0019	1.001 21	1.583 66
μ_g	0.40323	0.41897	0.43768	0.45372	0.4493	0.44407	0.41757	0.410586	0.51079
E2 (eV)	1.5953	0.10014	0.50200	0.35017	0.14561	0.13001	0.90061	1.599 27	0.10878
	(110)	(111)	(112)	(113)	(114)	(115)	(116)	(117)	(118)
<i>b</i> 1	1.5	1.7	1.7	2.0	2.0	2.0	2.0	2.3	2.5
_3\									
$n_0 \text{ (cm}^{-3})$	10^{17}	10^{16}	10^{16}	10^{17}	10^{16}	5×10^{9}	10^{16}	10^{16}	10^{18}
$n_0 \text{ (cm}^{-3})$ $N \text{ (cm}^{-3})$	10^{17}	10^{16}	10^{16}	$10^{17} \\ 10^{18}$	10^{16} 10^{16}	10^{18}	10^{16}	10^{16}	10^{18}
$n_0 \text{ (cm}^{-3})$ $N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$				10^{18} 3×10^9					
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV)	10^{17}	10^{16}	10^{16}	10^{18}	10^{16}	10^{18}	10^{16}	10^{16}	10^{18}
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$	10 ¹⁷ 10 ³	10^{16} 10^{13}	10 ¹⁶ 10 ⁵	10^{18} 3×10^9	10 ¹⁶ 10 ⁴	10^{18} 10^{11}	10^{16} 10^4	10 ¹⁶ 10 ¹³	10^{18} 10^{17}
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV)	10 ¹⁷ 10 ³ 0.1	10 ¹⁶ 10 ¹³ 1.6	10 ¹⁶ 10 ⁵ 0.1	10^{18} 3 × 10 ⁹ 0.8	10 ¹⁶ 10 ⁴ 0.1	$ \begin{array}{c} 10^{18} \\ 10^{11} \\ 0.316 \end{array} $	10 ¹⁶ 10 ⁴ 0.1	10 ¹⁶ 10 ¹³ 1.6	10 ¹⁸ 10 ¹⁷ 2.0
N (cm ⁻³) S (s ⁻¹) E1 (eV) R (K s ⁻¹)	10 ¹⁷ 10 ³ 0.1 0.5	10 ¹⁶ 10 ¹³ 1.6 0.5	10 ¹⁶ 10 ⁵ 0.1 0.5	10^{18} 3×10^{9} 0.8 0.2	10 ¹⁶ 10 ⁴ 0.1 0.2	10 ¹⁸ 10 ¹¹ 0.316 2.0	10 ¹⁶ 10 ⁴ 0.1 0.5	10 ¹⁶ 10 ¹³ 1.6 0.5	10 ¹⁸ 10 ¹⁷ 2.0 2.0
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV) $R \text{ (K s}^{-1})$ $A_1 \text{ (a.u.)}$	10 ¹⁷ 10 ³ 0.1 0.5 26 031.30	10 ¹⁶ 10 ¹³ 1.6 0.5 21 452.3	10 ¹⁶ 10 ⁵ 0.1 0.5 87 466.8	10^{18} 3×10^{9} 0.8 0.2 87510.3	10 ¹⁶ 10 ⁴ 0.1 0.2 354782	10 ¹⁸ 10 ¹¹ 0.316 2.0 44 058.9	10 ¹⁶ 10 ⁴ 0.1 0.5 22 206.3	10 ¹⁶ 10 ¹³ 1.6 0.5 44 042.6	10 ¹⁸ 10 ¹⁷ 2.0 2.0 176 826
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV) $R \text{ (K s}^{-1})$ $A_1 \text{ (a.u.)}$ $A_m \text{ (a.u.)}$	10 ¹⁷ 10 ³ 0.1 0.5 26 031.30 15 351.80	10 ¹⁶ 10 ¹³ 1.6 0.5 21 452.3 12 388.3	10 ¹⁶ 10 ⁵ 0.1 0.5 87 466.8 52 645.2	10^{18} 3×10^{9} 0.8 0.2 87510.3 54036.1	10 ¹⁶ 10 ⁴ 0.1 0.2 354782 224638	10 ¹⁸ 10 ¹¹ 0.316 2.0 44 058.9 28 402.7	10 ¹⁶ 10 ⁴ 0.1 0.5 22 206.3 14 149.2	10 ¹⁶ 10 ¹³ 1.6 0.5 44 042.6 27 794.1	10 ¹⁸ 10 ¹⁷ 2.0 2.0 176 826 113 512
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV) $R \text{ (K s}^{-1})$ $A_1 \text{ (a.u.)}$ $A_m \text{ (a.u.)}$ $A_2 \text{ (a.u.)}$	10 ¹⁷ 10 ³ 0.1 0.5 26 031.30 15 351.80 4413.33	10 ¹⁶ 10 ¹³ 1.6 0.5 21 452.3 12 388.3 3540.42	10 ¹⁶ 10 ⁵ 0.1 0.5 87 466.8 52 645.2 15 934.9	10^{18} 3×10^{9} 0.8 0.2 87510.3 54036.1 17251.8	10 ¹⁶ 10 ⁴ 0.1 0.2 354782 224638 7602.19	10 ¹⁸ 10 ¹¹ 0.316 2.0 44 058.9 28 402.7 9858.06	10 ¹⁶ 10 ⁴ 0.1 0.5 22 206.3 14 149.2 4869.78	10 ¹⁶ 10 ¹³ 1.6 0.5 44 042.6 27 794.1 9336.26	10 ¹⁸ 10 ¹⁷ 2.0 2.0 176 826 113 512 39 251.3
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV) $R \text{ (K s}^{-1})$ $A_1 \text{ (a.u.)}$ $A_m \text{ (a.u.)}$ $A_2 \text{ (a.u.)}$ $T_1 \text{ (K)}$	10 ¹⁷ 10 ³ 0.1 0.5 26 031.30 15 351.80 4413.33 100.16	10 ¹⁶ 10 ¹³ 1.6 0.5 21 452.3 12 388.3 3540.42 529.16	10 ¹⁶ 10 ⁵ 0.1 0.5 87 466.8 52 645.2 15 934.9 74.310	10 ¹⁸ 3 × 10 ⁹ 0.8 0.2 87 510.3 54 036.1 17 251.8 362.16	10 ¹⁶ 10 ⁴ 0.1 0.2 354782 224638 7602.19 80.110	10 ¹⁸ 10 ¹¹ 0.316 2.0 44 058.9 28 402.7 9858.06 334.56	10 ¹⁶ 10 ⁴ 0.1 0.5 22 206.3 14 149.2 4869.78 84.76	10 ¹⁶ 10 ¹³ 1.6 0.5 44 042.6 27 794.1 9336.26 526.86	10 ¹⁸ 10 ¹⁷ 2.0 2.0 176 826 113 512 39 251.3 540.76
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV) $R \text{ (K s}^{-1})$ $A_1 \text{ (a.u.)}$ $A_m \text{ (a.u.)}$ $A_2 \text{ (a.u.)}$ $T_1 \text{ (K)}$ $T_m \text{ (K)}$	10 ¹⁷ 10 ³ 0.1 0.5 26031.30 15351.80 4413.33 100.16 114.827	10 ¹⁶ 10 ¹³ 1.6 0.5 21 452.3 12 388.3 3540.42 529.16 554.96	10 ¹⁶ 10 ⁵ 0.1 0.5 87 466.8 52 645.2 15 934.9 74.310 82.560	10^{18} 3×10^9 0.8 0.2 87510.3 54036.1 17251.8 362.16 387.16	10 ¹⁶ 10 ⁴ 0.1 0.2 354782 224638 7602.19 80.110 90.110	10 ¹⁸ 10 ¹¹ 0.316 2.0 44 058.9 28 402.7 9858.06 334.56 389.96	10 ¹⁶ 10 ⁴ 0.1 0.5 22 206.3 14 149.2 4869.78 84.76 95.96	10 ¹⁶ 10 ¹³ 1.6 0.5 44 042.6 27 794.1 9336.26 526.86 554.46	10 ¹⁸ 10 ¹⁷ 2.0 2.0 176 826 113 512 39 251.3 540.76 564.46
$N \text{ (cm}^{-3})$ $S \text{ (s}^{-1})$ E1 (eV) $R \text{ (K s}^{-1})$ $A_1 \text{ (a.u.)}$ $A_m \text{ (a.u.)}$ $A_2 \text{ (a.u.)}$ $T_1 \text{ (K)}$ $T_m \text{ (K)}$ $T_2 \text{ (K)}$	10 ¹⁷ 10 ³ 0.1 0.5 26 031.30 15 351.80 4413.33 100.16 114.827 129.827	10 ¹⁶ 10 ¹³ 1.6 0.5 21 452.3 12 388.3 3540.42 529.16 554.96 579.96	10 ¹⁶ 10 ⁵ 0.1 0.5 87 466.8 52 645.2 15 934.9 74.310 82.560 91.260	10^{18} 3×10^9 0.8 0.2 87510.3 54036.1 17251.8 362.16 387.16 414.76	10 ¹⁶ 10 ⁴ 0.1 0.2 354782 224638 7602.19 80.110 90.110 101.71	10 ¹⁸ 10 ¹¹ 0.316 2.0 44 058.9 28 402.7 9858.06 334.56 389.96 456.96	10 ¹⁶ 10 ⁴ 0.1 0.5 22 206.3 14 149.2 4869.78 84.76 95.96 108.96	10 ¹⁶ 10 ¹³ 1.6 0.5 44 042.6 27 794.1 9336.26 526.86 554.46 586.26	10 ¹⁸ 10 ¹⁷ 2.0 2.0 176 826 113 512 39 251.3 540.76 564.46 592.76

than the symmetry factor for estimating the value of the order of kinetics b.

As a test case of the present work, we have taken an isolated 282 °C TL glow peak of the 1.0 rad 60 Co gamma-irradiated CaF₂:Mn, figure 4. The experimental details can be found elsewhere [47]. The areas A_i under the glow peak between T_i and T_f are calculated. The following data are obtained from the glow curve of figure 4, and used to calculate the trapping parameters: $T_1 = 518.33 \pm 1.23$ K, $T_m = 555.16 \pm 1.23$ K and $T_2 = 582.46 \pm 1.23$ K; $A_1 = 57.288 \pm 1920$, $A_m = 28.005 \pm 1330$ and $A_2 = 5539 \pm 925$ (in arbitrary units).

The order of kinetics b obtained from equation (19) is $1.001\,61\pm0.093\,66$. The activation energy E (eV) is obtained after evaluating the order of kinetics b using equation (17) or (18), $E=0.948\,95\pm0.0265$ eV. The frequency factor S (s⁻¹) is calculated according to equation (20), $S=(1.856\pm1.079)\times10^7$ s⁻¹. The theoretical peak with $b=1.001\,61\pm0.093\,66$, $E=0.948\,95\pm0.0265$ eV, $S=(1.856\pm1.079)\times10^7$ s⁻¹ and the heating rate R=1.25 K s⁻¹ fits well to the experimental one as shown in figure 4.

The advantage of the present method is that it directly gives the exact value of the order

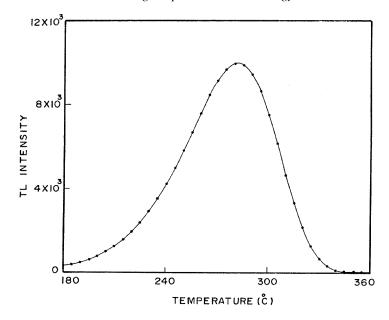


Figure 4. Isolated 282 °C TL glow peak of 1.0 rad 60 Co gamma-irradiated CaF₂:Mn [47]. Solid line, experimental peak; points, numerically generated peak with $b=1.001\,61\pm0.093\,66$, $E=0.948\,95\pm0.0265$ eV, $S=(1.856\pm1.079)\times10^7$ s⁻¹ and R=1.25 K s⁻¹.

of kinetics b and the activation energy E and the present method is appreciably simpler than the graphical method mentioned by Chen [3]. We suggest that one should estimate the order of kinetics b from equation (19) and use it to estimate the activation energy E using equations (17) or (18) and finally use these two parameters to fit the experimental peak to a numerically computed one.

5. Conclusion

The most important method for obtaining the order of kinetics b is the symmetry factor μ_g . The difficulties with respect to using the symmetry factor for obtaining the order of kinetics are demonstrated during this work. As a result an equation is derived which gives the order of the first-, second- or general-order glow peak in terms of its peak temperature T_m , T_1 , T_2 and the peak areas A_m , A_1 and A_2 . Also, the activation energy E (eV) can be obtained after evaluating the order of kinetics b using the maximum intensity A_m and T_m (K).

The validity of this method is examined for a broad range of values of kinetic orders. The applicability of the present method is demonstrated by taking some numerically computed general-order TL glow peaks.

References

- [1] Randall J T and Wilkins M H F 1945 Proc. R. Soc. A 184 366
- [2] Garlick G F J and Gibson A F 1948 Proc. Phys. Soc. 60 574
- [3] Chen R 1969 J. Electrochem. Soc. 116 1254
- [4] Rasheedy M S 1993 J. Phys.: Condens. Matter 5 633
- [5] Halperin A and Braner A A 1960 Phys. Rev. 117 408
- [6] Kathura S P and Sunta C M 1982 J. Phys. D: Appl. Phys. 15 497

- [7] Kathura S P and Moharil S V 1983 J. Phys. D: Appl. Phys. 16 1331
- [8] Ahmed A B and Gartia R K 1985 Phys. Status Solidi a 89 231
- [9] Jain V K and Jahan M S 1985 Phys. Status Solidi a 92 237
- [10] Takeuchi N, Ohtaki K and Nakamura S 1985 Phys. Status Solidi a 130 K145
- [11] Azorin J, Gutierrez A and Martinez C G 1985 Radiat. Eff. 84 263
- [12] Azorin J 1986 Nucl. Tracks 11 159
- [13] Azorin J and Gutierrez A 1986 Nucl. Tracks 11 167
- [14] Gartia R K, Singh S J and Ahmed A B 1987 Phys. Status Solidi a 103 593
- [15] Campos L L 1988 Appl. Radiat. Isot. 39 233
- [16] Ramana M V and Sastry G S 1989 Phys. Status Solidi a 116 K205
- [17] Azorin J, Furuta C and Gutierrez A 1989 J. Phys. D: Appl. Phys. 22 458
- [18] Moharil S V, Patey S M and Deshmukh B T 1989 J. Lumin. 42 325
- [19] Takeuchi N 1983 Phys. Status Solidi a 78 K93
- [20] Christodoulides C 1985 J. Phys. D: Appl. Phys. 18 1501
- [21] Opanowicz A 1987 Phys. Status Solidi b 101 589
- [22] Gartia R K, Singh S J and Mazumdar P S 1988 Phys. Status Solidi a 106 291
- [23] Opanowicz A 1989 Phys. Status Solidi a 116 343
- [24] Christodoulides C 1990 Phys. Status Solidi a 118 333
- [25] Balarin M 1975 Phys. Status Solidi a 31 K111
- [26] Gartia R K and Singh S J 1992 Phys. Status Solidi a 132 197
- [27] May C E and Partridge J A 1964 J. Chem. Phys. 40 1401
- [28] Partridge J A and May C E 1965 J. Chem. Phys. 42 797
- [29] Muntoni C, Rucci A and Serpi P 1968 Ricerea Sci. 38 762
- [30] Ward R W and Whippey P W 1971 Can. J. Phys. 50 1409
- [31] Ausin V and Alvarez-Rivas J L 1972 J. Phys. C: Solid State Phys. 5 82
- [32] Macciota-Serpi P, Rucci A and Serpi A 1975 J. Lumin. 9 488
- [33] Takeuchi N, Inabe K and Nanto H 1975 Solid State Commun. 17 1267
- [34] Chen R 1984 Thermoluminescence and Thermoluminescent Dosimetry vol 1, ed Y S Horowitz (Boca Raton, FL: Chemical Rubber Company)
- [35] Moharil S V 1981 Phys. Status Solidi a 66 767
- [36] Moharil S V 1981 Phys. Status Solidi a 68 413
- [37] Moharil S V 1982 Phys. Status Solidi a 73 509
- [38] Moharil S V 1984 J. Phys. D: Appl. Phys. 17 2301
- [39] Chen R 1969 J. Appl. Phys. 40 570
- [40] Shalgaonkar C S and Narlikar A V 1972 J. Mater. Sci. 7 1465
- [41] Chen R 1976 J. Mater. Sci. 11 1521
- [42] Chen R and Kirsh Y 1981 Analysis of Thermally Stimulated Processes vol 15 (Oxford: Pergamon)
- [43] McKeever S W S 1985 Thermoluminescence of Solids (Cambridge: Cambridge University Press)
- [44] Rasheedy M S and Amry A M 1994 Phys. Status Solidi a 142 K47
- [45] Rasheedy M S and Amry A M 1995 J. Lumin. 63 149
- [46] Srivastava J K and Supe S J 1979 Nucl. Instrum. Methods 160 529
- [47] Hornyak W F, Levy P W and Kierstead J A 1985 Nucl. Tracks 10 557