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Computerised glow curve deconvolution (CGCD) : the case of TLD-300

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Abstract Computerised glow curve deconvolution (CGCD) in principle can provide meaningful and unique trapping parameters provided one uses the correct model in simulating the numerical glow peaks. In the absence of the knowledge of the exact model, simple models like the one used in kinetics formalism can still yield trapping parameters defined at least semiquantitatively. This has been shown by deconvoluting three glow curves (two due to γ and one due to α-irradiation) of TLD-300 (CaF_2 : Tm)

The importance of peak finding by second derivative plot of the glow curve is demonstrated. It has been found that all the glow peaks do not follow first order kinetics.

Keywords Thermoluminescence (TL), activation energy, figure of merit (FOM)

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1. Introduction

Computerised glow curve deconvolution (CGCD) technique is now widely used in various areas of thermoluminescence (TL) studies and is well documented [1,2]. At the present state of development, CGCD in general, is performed in the framework of kinetics formalism [3-5].

In this paper, we would like to discuss the application of CGCD in establishing the trapping parameters of TLD-300 (CaF_2 : Tm). The selection of the material is based on the fact that a number of workers have applied CGCD to the glow peaks of this material [6-8]. Further, ever since its introduction to the family of TLDs [9], the material remains a candidate in mixed radiation field dosimetry on the ground that its major peaks, namely 3 and 5, show different response to linear energy transfer (LET : defined as dE/dl where dE is the energy loss by a charged particle travelling a distance dl, due to collisions) of the radiation.

Our study is based on CGCD of two glow curves of TLD-300, one irradiated by γ-rays and the other by α-rays. The data are taken from the paper of Olko [10]. We have performed CGCD on a glow curve of Bos and Dielhof [8] as well, not only to check our deconvolution technique but to establish the trapping parameters of the glow peaks at least semiquantitatively. The CGCD software used in the present work is essentially the one presented in the book of Chen and Kirsh [11]. The only modification incorporated is the selection of the peak temperature (Tm) within ± 1°C. The criterion for the best fit with a specific set of the activation energy (E), the frequency factor (s), the order of kinetics (b) is judged from the minimum value of the root mean square deviations.

2. Results and discussion

The results of CGCD of the glow curves of TLD-300 are shown in Figures 1 and 2. The goodness of fit is checked by the value of the Figure of Merit (FOM) which is defined as follows :

$$\mathrm{FOM} = \sum^{j_{stop}} \quad - y(x_j) \quad \times 100,$$

where

FOM	=	Figure of Merit in per cent,
j_{start}	=	first channel in fitting region,
j_{stop}	=	last channel in fitting region,
y_j	=	content of channel j,
$y(x_j)$	=	value of fitting function in the middle of channel j,
A	=	the integral of the fitted glow curve.

The FOM first proposed by Misra and Eddy [12] has become not only popular but acceptable by the community of CGCD workers where FOM values of a few percent is taken as an acceptable fit [13]. In both cases, the fitting is good in the sense that for γ-irradiated glow curve the FOM = 0.03068% whereas that for α-irradiated one FOM = 0.01367%. The values of the trapping parameters for the best-fit deconvoluted constituent peaks are presented in Table 1. Unlike the case of Bos and Dielhof [8] our results show that not all peaks do follow first order kinetics.

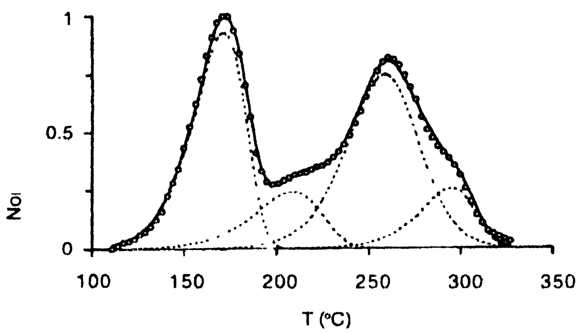

Figure 1. CGCD results of γ-irradiated glow curve of TLD-300 of Olko [10]. The FOM value obtained is 0.03068% o o o – Experimental data. --- Best-fit glow peaks. — Sum of best-fit glow peaks

In an attempt to lend further support to our result we have plotted the second derivative of the γ-irradiated glow curve which is supposed to reveal four negative peaks each corresponding to one of the four glow peaks. The result is shown in Figure 3 along with the deconvoluted best-fit peaks. There is a close agreement between the peak temperature with that of the negative peaks of second derivative plot of the glow curve. This result provides physical basis to the location of glow peak temperature (Tm), a point not checked in CGCD.

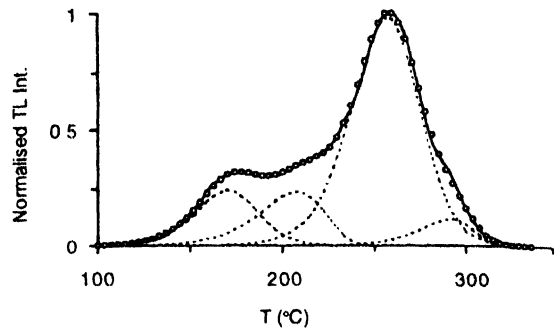

Figure 2. CGCD results of α-irradiated glow curve of TLD-300 of Olko [10]. The FOM value obtained is 0.01367%. o o o – Experimental data --- Best-fit glow peaks — Sum of best-fit glow peaks

Table 1. CGCD result of TLD-300 (CaF, Tm)

Glow peak	T_m (°C)	E(eV)	$s(s^{-1})$	Order of kinetics	Ref Glow curve
1	088 00	0 740	1.4×10^{9}	1	Bos & Dielhof [8]
		1.00 ± 0.07	1.0×10^{13}		*
2	110 79	1 036	3.3×10^{12}	1	Bos & Dielhof [8]
		1.08 ± 0 09	3.0×10^{13}		*
	171.38	1.198	5.4×10^{12}	1	γ-irradiated, Olko [10]
3	170 48	1.186	4.1×10^{12}	1 5	α-irradiated, Olko [10]
	152 01	1 132	1.9×10^{12}	1	Bos & Dielhof [8]
		1.22 ± 0.04	$(3 \pm 2) \times 10^{13}$		*
	208.86	1.051	1.0×10^{11}	1	γ-irradiated, Olko [10]
4	207 72	1.079	2.2×10^{11}	1	α-irradiated, Olko [10]
	192.65	1 199	6.1×10^{11}	1	Bos & Dielhof [8]
		1.37 ± 0.03	$(7 \pm 4) \times 10^{13}$		*
	258.98	1 528	3.7×10^{13}	1 5	γ-irradiated, Olko [10]
5	256 95	1.592	1.8×10^{14}	1.5	α-irradiated, Olko [10]
	239.98	1.583	2.4×10^{14}	1.5	Bos & Dielhof [8]
		1.74 ± 0.04	$(1.3 \pm 0.6) \times 10^{14}$		*
	295.00	1 821	1.9×10^{15}	1	γ-irradiated, Olko [10]
6	291.59	1.890	1.0×10^{16}	1	α-irradiated, Olko [10]
	275.40	1 951	6.4×10^{16}	1	Bos & Dielhof [8]
		1.88 ± 0 02	$(5 \pm 3) \times 10^{16}$		*

* Result of Bos & Dielhof [8] (Various heating rates method)

In order to lend further support to our CGCD results, we have applied the technique to a glow curve of Bos and Dielhof

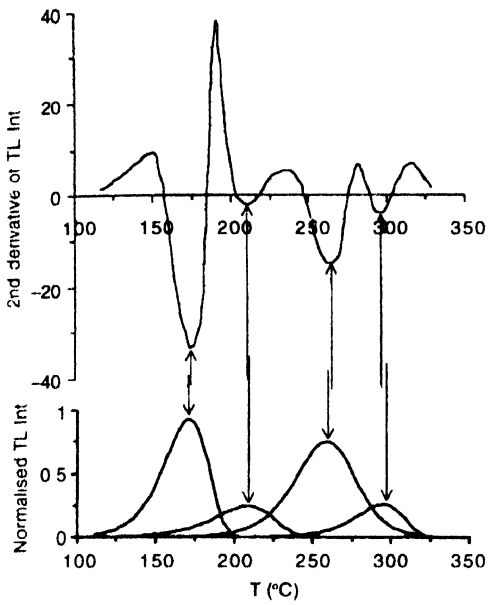

Figure 3. Second derivative plot of the glow curve (Figure 1) along with the best fit glow peaks.

[8] (Figure 4). The results of the deconvolution are presented in Table 1 for comparison. The results are in good agreement. Further, the plot of the second derivative of the glow curve along with the peak temperature of the best fit glow curves (as

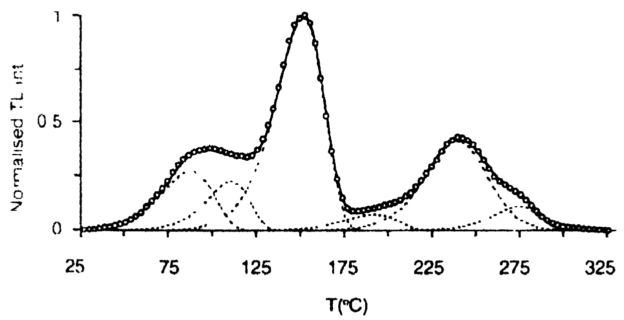

Figure 4. CGCD results of γ-irradiated glow curve of TLD-300 of Bos and Dielhof [8]. The FOM value obtained is 0.02341%. o o o – Experimental data --- Best-fit glow peaks. — Sum of best-fit glow peaks

obtained by us) shows very good correlation justifying the present analysis (Figure 5). In the same figure, the Tm's of the deconvoluted peaks reported by Bos and Dielhof [8] are also marked which shows that the location of the 2nd and 6th peak differ by 6°C and 17°C when compared to negative maxima of the second derivative plot.

3. Conclusion

Thus we conclude that

i) Not all the glow peaks of TLD-300 follow first order kinetics.

ii) In the process of fitting, the entire glow curve of TLD-300 to first order peaks Bos and Dielhof [8] have failed to locate the exact glow peak temperatures. This has resulted in the large discrepancy between the VHR and CGCD results for the 2nd and 6th peak.

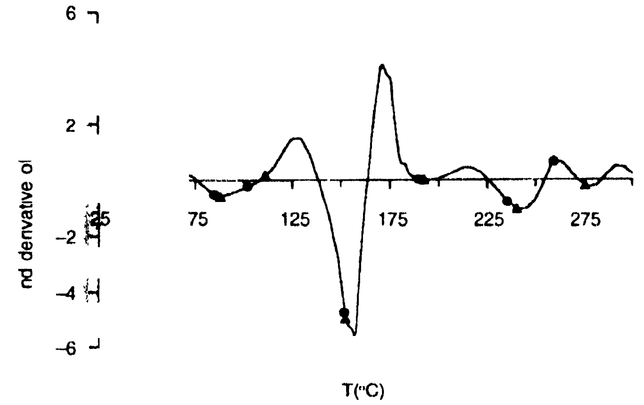

Figure 5. Second derivative plot of the glow curve (Figure 4) along with peak temperature (Tm) markers ▲▲▲ - Tm's of present deconvolution ●●● - Tm's reported by Bos and Dielhof [8]

iii) Even when the fit between the experimental and numerically generated curve is deceptively precise, CGCD does not guarantee meaningful data.

iv) The second derivative plot of a glow curve can guide one to locate the glow peak temperatures

v) Kinetics formalism may not be the exact model but it gives a fairly good mathematical description of the phenomena, use of which in CGCD can provide trapping parameters reliable at least semiquantitatively. Thus, one can measure the areas of peaks 3 and 5 accurately by resorting to CGCD which will provide valuable information on the radiation quality in mixed radiation fields.

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