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Kinetic Analysis of Computer Programmed Deconvoluated Thermoluminescence Glow Curves of LiF: Mg, Ti (TLD-100)

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ABSTRACT

Thermoluminescence glow curve technique is widely used for characterization of materials for dosimetry as well as for dating purpose. Computerized glow curve deconvolution is widely used for studying the thermoluminescence mechanism as well as for thermo luminescence dosimetry. Chung et. al., have developed a quick and efficient programme to resolve different peaks in thermo luminescence glow curve of LiF:Mg,Ti (TLD-100), which is a standard TL material. In present work we evaluate order of kinetics involved in these different peaks. The method for evaluation of order of kinetics used here depends on new mechanism suggested for appearance of thermoluminescence glow curve.

Keywords: ***Glow Curve Dconvolution, Thermoluminescence, Order of Kinetics.***

INRODUCTION:

Thermoluminescence (TL) is an important and convenient tool for determination of trap energy and escape frequency factor. Mostly TL studies of specimen of different material have multiple peaks. For determination of trap parameters it is necessary to resolve these peaks. Over the last three decades computerized deconvolution of TL glow curves has became the method of choice for TL glow curve analysis. In order to resolve multiple peaks, for analysis of glow curves, Computerized Glow Curve Deconvolution (CGCD) method is widely used and nowadays also used in routine radiation dosimetry. CGCD technique for the decomposition of a composite of a composite TL glow curve into its individual glow peaks is firstly applied by Horowitz *et.al.* [1]. Several mechanisms, models and approximations and minimization procedures have been investigated and a number of computer programs [2, 3] have been developed for TL glow curve analysis. An important step in establishing deconvolution as a reliable research tool was the GLOCANIN project [4,5,6] – an intercomparison of glow curve analysis programs.

MECHANISM AND METHOD OF ANALYSIS:

There are so many models are suggested by different workers for appearance of glow curve and correspondingly there are different methods, as reported in literature, for the analysis of TL glows curve or spectrum. Mechanisms, on which the above methods of analysis of TL glow curve are based, have some anomalies like different analysis method for different kinetics order insufficient equation for peak temperature.

In order to remove above shortcomings of previous suggested mechanisms Prakash [7] has suggested a new model for appearance of TL glow curve by reconsidering the basic idea of Adirovitch [8]. A simple model has been proposed which explains the mechanisms involved in the occurrence of TL glow curve. Out of the electrons

excited to the conduction band, some are re-trapped and balance gets recombined in such a way that the sum of re-trapped and recombined electrons is equal to the electrons excited to the conduction band. In this model it is suggested that order of kinetics involved in TL process depends on extent of re-trapping ***x***. The general equation for intensity of TL glow curve having any extent of re-trapping is given by [7]

$$I = (1 - \boldsymbol{x}) n_o s \exp\left[-\frac{E_a}{k\,T} - \frac{s\,(1-\boldsymbol{x})}{b}\int_{T_o}^{T} \exp\left(-\frac{E_a}{k\,T'}\right) dT'\right] \qquad (1)$$

where n_0 is initial concentration of trapped electrons per unit volume at temperature T_o, T_o is initial temperature wherefrom TL glow curve starts to appear, s is pre-exponential or escape frequency factor, E_a is activation energy or trap depth,, k is Boltzmann's constant, T the absolute temperature, b the constant linear heating and T' an arbitrary temperature in the range T_o to T. Extent of re-trapping x is related with order of kinetics ℓ by relation

$$\ell = \frac{1}{(1-\boldsymbol{x})} \qquad (2)$$

Equation for peak temperature is given by

$$T_m^2 = \frac{b\,E_a\,\tau_m}{(1-\boldsymbol{x})k} \qquad (3)$$

or in terms of order of kinetics

$$T_m^2 = \frac{\ell\,b\,E_a\,\tau_m}{k} \qquad (4)$$

Where τ_m is relaxation time at peak temperature T_m given by Arrhenius relation [9]

$$\tau_m = \tau_o \exp\left[\frac{E_a}{kT_m}\right] \qquad (10)$$

Where τ_0 is fundamental relaxation time and is inverse of escape frequency factor s.

Depending above suggested model for appearance of TL glow curve, analysis method for glow curve is suggested by Prakash [7] and coworkers. This method is simply BFG [10] method in which kinetics idea is introduced. Following this method of analysis to calculate the different trapping parameters it is necessary to resolve all the peaks of glow curve.

In order to resolve overlapping peaks of glow curve, Chung *et. al.* [11] have developed a quick and efficient computer program. This computerized glow curve deconvolution programe is tested by Chung et al on standard TL materials such as LiF:Mg,Ti (TLD-100) or MCP-N which are most intensively studied. TLD-100 is most popular and commonly used dosimeter even though it is very complex material.

ANALYSIS RESULT:

Data presented by Chung et al for TLD-100 material deconvoluted for first order kinetics model is presented in Table 1. Data in column 1 and 2 are presented as such. The values of τ_0, i.e.,

Table.1
Different parameters of the glow peaks TLD-100 deconvoluted for first order kinetics

Peak No.	E_a (eV)	τ_0 (s)	T_m (K)	T_m^2 (K^2)	$(bE_a\tau_m)/k$	ℓ
2	0.99	9.09E-13	383.3333	146944.4	108433.8	1.355153
3	1.17	1.69E-13	423.3333	179211.1	195592.5	0.916247
4	1.88	1.63E-20	453.3333	205511.1	283867.2	0.723969
5	2.00	1.08E-20	480.0000	230400.0	251397.0	0.916479
6	2.25	7.09E-23	490.0000	240100.0	257241.4	0.933364
7	0.83	3.45E-07	533.3333	284444.4	231623.2	1.228048

Fundamental relaxation time for different peaks, are calculated from given value of escape frequency factor. Peak temperature values for different peaks are measured from resolved peaks of deconvoluted curve as reported by Chung et al [11]. Linear heating rate b during TL process and is 1^0K/s. Before mechanism proposed by Prakash [7] relation used for peak temperature is [12]

$$T_m^2 = \frac{b\,E_a\tau_m}{k} \qquad (11)$$

Both L.H.S. and R.H.S. of eq. (11) are calculated from reported values, and are shown in columns 5 and 6 of Table.1. It is clear that they are not equal. This anomaly is also removed in model proposed by Prakash and coworkers. The peak temperature eq. (11) is modified in eq.(4) and accordingly evaluated kinetics values are presented in column 7 of Table.1.

Table.2
Different parameters of the glow peaks TLD-100 adapted from Horowitz et al [1]

Peak No.	E_a (eV)	τ_0 (s)	T_m (K)	T_m^2 (K^2)	$(bE_a\tau_m)/k$	ℓ
2	1.26	5.88E-16	383.3333	146944.4	316765.6	0.46389
3	1.33	1.54E-15	423.3333	179211.1	162116.9	1.105443
4	1.62	1.32E-07	453.3333	205511.1	2.53E+15	8.11E-11
5	2.12	6.67E-22	480.0000	230400.0	298380.0	0.77217

Table.3
Different parameters of the glow peaks TLD-100 deconvoluted for GOK

Peak No.	E_a (eV)	τ_0 (s)	T_m (K)	T_m^2 (K^2)	$(bE_a\tau_m)/k$	ℓ
2	1.36	1.03E-17	383.3333	146944.4	123315.6	1.191613
3	1.07	2.65E-12	423.3333	179211.1	180038.6	0.995404
4	1.83	5.24E-20	453.3333	205511.1	246176.8	0.834811
5	2.09	1.10E-21	480.0000	230400.0	234249.3	0.983568
6	2.53	9.71E-26	490.0000	240100.0	300362.3	0.799368
7	0.80	6.25E-06	533.3333	284444.4	2106559	0.135028

Similarly, τ_0, T_m, $(bE_a\tau_m)/k$ and ℓ are calculated from reported values of E_a and s. In Table.2 values are taken from Horowitz et al [1]. In Table.3 values of b, E_a and s are taken from TL glow curve of TLD-100 deconvoluted for general order kinetics (GOK) and in Table.4 known parameters are taken from TL glow curve of TLD-100 deconvoluted for general approximation (GA). Order of kinetics ℓ is evaluated for both cases GOK and GA.

Table.4
Different parameters of the glow peaks TLD-100 deconvoluted for first GA

Peak No.	E_a (eV)	τ_0 (s)	T_m (K)	T_m^2 (K^2)	$(bE_a\tau_m)/k$	ℓ
2	1.14	8.70E-15	383.3333	146944.4	112019.2	1.311779
3	1.18	1.16E-13	423.3333	179211.1	177396.1	1.010231
4	1.85	2.97E-20	453.3333	205511.1	235354.8	0.873197
5	1.99	1.37E-20	480.0000	230400.0	248689.8	0.926455
6	2.25	5.21E-23	490.0000	240100.0	188911.7	1.270964
7	1.47	2.87E-16	533.3333	284444.4	380.6814	747.1982

COCLUSION:

An efficient computer deconvoluted programe for TLD-100 is suggested by Chung et al. All the overlapping peaks are properly resolved with this programe. Considering values of escape frequency factor, activation energy, linear heating rate and peak temperature values for different resolved peaks from reported data of Chung and Horowitch, fundamental relaxation time, square of peak temperature $(bE_a\tau_m)/k$ are evaluated. It is found that in general eq.(5) is not satisfied. With the help of new method of analysis, order of kinetics are evaluated for all the six curves of Li:Mg,Ti (TLD-100). Evaluated values of various parameters are quite helpful in studying TL as well as dosimetric characteristics of material under consideration.

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