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Development of the peak fitting and peak shape methods to analyze the thermoluminescence glow-curves generated with exponential heating function

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ABSTRACT

The general-semi analytical thermoluminescence (TL) expressions based on the one trap–one recombination center (OTOR) were developed to fit the single glow-peaks generated with exponential heating function (EHF) profile. The peak shape method (PSM) expressions based on the general-order kinetics (GOK) model were also developed for the glow-peaks generated with EHF profile. The success and failure of the GOK model in describing the glow-peaks generated with EHF was discussed. The new developed TL expressions were tested in the cases in which the other TL expressions based on the GOK model failed. The results showed that in the case of dose saturation and strong re-trapping probability, the error in the calculated activation energy (E) using the GOK model expressions exceeded 50%. While, using the new developed TL expressions, the error in the calculated E did not exceed 0.5%.

1. Introduction

The thermoluminescence (TL) dosimeters used with exponential heating function (EHF) profile are characterized by high reproducibility, nearly constant black-body radiation contribution and short time needed to record its TL glow-curves [1]. However, their glow-curves are characterized by a relatively poor resolution of their individual glow-peaks, making the methods of determining the kinetics parameters a difficult task [2]. The shape of a TL glow-peak is the basis of important and convenient methods for calculating the kinetics parameters [3].These parameters can be determined using the peak fitting or the peak shape methods. Unfortunately, the existing peak shape method (PSM) expressions were deduced only for the glow-peaks generated with linear heating function (LEF) profile. However, some investigators [2,4,5] have applied the peak fitting method, assuming the LHF profile, to the glow curves recorded with EHF profile. Later, it was concluded by Kitis et al. [6,7] that this assumption is not accurate.

Therefore, the former authors derived single glow-peak expressions for the peak fitting method to analyze the TL glow-curves recorded with EHF profile. These expressions were used in the analysis of very different glow-curves [8]. However, these expressions are based on the first- and the general-order kinetics (GOK) models. It was concluded [9–16] that these models fail to describe the glow peaks in the cases whenever the re-trapping probability becomes greater than the recombination one ($A_n \gg A_m$), and the sample dose is in the saturation range ($n_o = N$). Later, Kitis and Vlachos [17] deduced, using the Lambert-W function, semi-analytical expressions to describe the TL single glow-peak based on the one trap–one recombination center (OTOR) model. These expressions were tested in many different cases by Sadek et al. [16] and it was concluded that these expressions can, accurately, describe the TL glow peaks in the cases in which the other TL expressions were failed. Lovedy Singh and Gartia [18] also deduced the same expression, for $R < 1$ [19], except that they have used the Wright-ω function instead of the Lambert-W function. However, all these expressions were deduced only for the glow-peaks generated with LHF profile.

The aim of this work is to (a) develop the single glow-peak expressions deduced by Kitis and Vlachos [17] to fit the single glow-peaks generated with EHF profile, and (b) compare between the accuracy of the GOK model and the developed TL expressions in describing the glow-peaks generated with EHF. In order to

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achieve the second aim, the general-order kinetics PSM expressions were developed to be applicable for the glow-peaks generated with EHF profile.

2. The OTOR level model in the case of the exponential heating function (EHF)

The OTOR is based on a set of differential equations describing the transfer of charge carriers between a single trapping state, the conduction band and a single recombination state. In this model, the TL process consists of electrons released thermally from the electron traps into the conduction band from which they may either recombine with holes in the center or re-trap, namely fall back into the traps. However, there is no existing TL material known that accurately is described by the simple model. This does not mean that the simple model has no meaning. On the contrary, it can help us in the interpretation of many features which can be considered as variations of the OTOR model [20]. Halperin and Braner [21] wrote the set of three simultaneous differential equations governing the TL process for the OTOR model as follows:

$$\frac{dn}{dt} = -nS\exp\left(-\frac{E}{kT}\right) + n_c(N-n)A_n \tag{1}$$

$$\frac{dn_c}{dt} = nS\exp\left(-\frac{E}{kT}\right) - n_c(N-n)A_n - n_c m A_m \tag{2}$$

$$-\frac{dm}{dt} = n_c m A_m \tag{3}$$

where, A_m and A_n are the recombination and re-trapping probabilities in $(\mathrm{cm^3\ s^{-1}})$ respectively, N is the total concentration of trapping states in $(\mathrm{cm^{-3}})$, m, n, and n_c are the instantaneous concentrations of the holes in centers, the trapped charge carriers, and the electrons in the conduction band in $(\mathrm{cm^{-3}})$, E is the activation energy in (eV), S is the frequency factor in $(\mathrm{s^{-1}})$ and k is the Boltzmann constant in $\mathrm{eV\ K^{-1}}$. However, In the case of the EHF, the temperature (in K) of the solid as a function of time is given by [5]:

$$T(t) = T_g - (T_g - T_o)e^{-\alpha t} \tag{4}$$

where, T_g is the hot gas temperature approached asymptotically with time t, T_o is the temperature at $t = 0$, with α in $\mathrm{s^{-1}}$. Thus, the heating rate β will be given as:

$$\beta = \frac{dT}{dt} = \alpha(T_g - T) \tag{5}$$

Thus, the TL process in the case of the EHF can be described by the set of the differential equations Eqs. (1)–(3) along with Eq. (5).

3. Development of the TL expressions to describe a single glow-peak generated with EHF

Kits and Vlachos [17] deduced, using the Lambert-W function, single glow-peak expressions based on the OTOR model. However, these expressions were deduced only for the glow-peaks generated with LHF. Using the heating rate defined by Eq. (5), the TL expressions describing a single-glow peak generated with EHF will take the following form:

$$\text{For } A_n < A_m \quad I = \frac{NR}{(1-R)^2}\frac{S\exp\left(-\frac{E}{kT}\right)}{W[\exp(z1)] + W[\exp(z1)]^2} \tag{6}$$

$$\text{For } A_n > A_m \quad I = \frac{NR}{(1-R)^2}\frac{S\exp\left(-\frac{E}{kT}\right)}{W[-1,-\exp(-z2)] + W[-1,-\exp(-z2)]^2} \tag{7}$$

where W is the Lambert-W function, $R = A_n/A_m$, and

$$z1 = \frac{1}{c} - \ln(c) + \frac{Sn_oF(T,T_g,E)}{cNR\alpha}, \tag{8}$$

$$z2 = \frac{1}{|c|} + \ln(|c|) + \frac{Sn_oF(T,T_g,E)}{|c|NR\alpha}, \tag{9}$$

$$c = \frac{n_o(1-R)}{NR} \tag{10}$$

$$F(T,T_g,E) = \int_{T_o}^{T}\frac{\exp\left(-\frac{E}{kT}\right)}{T_g - T}dT = -\exp\left(-\frac{E}{kT_g}\right)Ei\left(\frac{E}{kT_g} - \frac{E}{kT}\right) + \left(-\frac{E}{kT}\right)\Bigg|_{T=T_o}^{T=T} \tag{11}$$

where Ei is the well known exponential integral and it is a MATLAB built-in function. Thus, there is no need to use its usual asymptotic approximation [22].

It is to be noted that the intensities I given by Eqs. (6) and (7) are functions of S, α, n_o, E, R, Tg, and c. However, the TL expressions of the form of $I(I_m, T_m, E, R, T_g, c)$ are highly desirable for the peak fitting method. The reason is that the peak maximum intensity and its corresponding temperature I_m, T_m, respectively, can be directly and accurately evaluated from the experimental glow-curve. In contrast, the parameters S, α, and n_o are unknown. Deducing the I as a function of I_m, T_m, E, R, T_g, and c is described below.

The condition of the peak maximum, according to Eqs. (6) and (7), is given by:

$$\frac{\beta_m E}{kT_m^2} = F_{TL}S\exp\left(-\frac{E}{kT_m}\right) \tag{12}$$

where, β_m is β defined by Eq. (5) at $T = T_m$ and,

$$F_{TL} = \frac{1}{1-R}\frac{2W[\exp(z1_m \text{ or } z2_m)] + 1}{(W[\exp(z1_m \text{ or } z2_m)] + 1)^2} \tag{13}$$

where $z1_m$(*or* $z2_m$) = $z1$(*or* $z2$) at $T = T_m$, respectively.

An investigation has been done for a broad range of activation energies ($0.7 \leqslant E \leqslant 2.0$ eV) and frequency factors ($10^7 \leqslant S \leqslant 10^{13}\ \mathrm{s^{-1}}$), which can be considered physically realistic [23], in order to cover all the values found thus far in various experiments. It was observed that, over the range of R from $10^{-3} \leqslant R \leqslant 10^{+3}$, the following relations hold:

$$\text{For } A_n < A_m, \quad F_{TL} = \frac{-1.54R^{2.5} + 1.05}{1-R} \tag{14}$$

$$\text{For } A_n > A_m, \quad F_{TL} = \frac{4.75R^{-0.35} - 4.2}{1-R} \tag{15}$$

Using the peak maximum condition given by Eq. (12), then Eqs. (8) and (9) will take the following form, respectively:

$$z1^{Appr} = \frac{1}{c} - \ln(c) + \frac{E(T_g - T_m)\exp\left(\frac{E}{kT_m}\right)F(T,T_g,E)}{(-1.54R^{2.5} + 1.05)kT_m^2} \tag{16}$$

$$z2^{Appr} = \frac{1}{|c|} + \ln(|c|) - \frac{E(T_g - T_m)\exp\left(\frac{E}{kT_m}\right)F(T,T_g,E)}{(4.75R^{-0.35} - 4.2)kT_m^2} \tag{17}$$

where $z1^{Appr}$ and $z2^{Appr}$ are the approximate expressions for $z1$ and $z2$ given by Eqs. (8) and (9), respectively. Then, the TL expressions, as a function of I_m, T_m, E, R, T_g, and c, describing a single glow-peak generated with EHF under the fundamental OTOR model are given by:

$$\text{For } A_n < A_m \quad I = I_m\exp\left(-\frac{E}{k}\left(\frac{1}{T} - \frac{1}{T_m}\right)\right)\frac{W\left[\exp\left(z1_m^{Appr}\right)\right]^2 + W\left[\exp\left(z1_m^{Appr}\right)\right]}{W\left[\exp\left(z1^{Appr}\right)\right]^2 + W\left[\exp\left(z1^{Appr}\right)\right]} \tag{18}$$