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Determination of Temperature Dependent Frequency Factor Constant from TL Glow Curves

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Abstract

A new method solely based on the theoretical and experimental analysis of thermoluminescence glow curves is proposed for the determination of the temperature dependent frequency factor constant.

1. Introduction

When a wide-band gap crystal is irradiated at room temperature by radiation, such as x-rays, γ-rays, β-rays, electrons are released from the valance band to the conduction band. These electrons are trapped at defect sites in the crystalline solid. Trapped electrons liberated by heat, which is usually done at a constant heating rate $dT/dt = \beta$, cross the conduction band and move to a luminescent center with the emission of light. This is called thermoluminescence (TL). The TL intensity is detected by a photomultiplier tube and a pulse counting system, and recorded as a function of time or temperature. The resulting curve is called a TL curve or "glow curve". Aside from its application in radiation dosimetry and to dating techniques in archaeology and geology, TL has proved useful for the study of lattice defects which act as "traps" to electrons and holes.

The analysis of TL glow curve gives the physical parameters of the traps, namely, the trap depth E, which is the vertical separation between the trap and the conduction band, the frequency factor s, which is the probability per second for the release of a trapped charge carrier. Various experimental techniques have been developed to determine these parameters from TL glow curves [1-5]. Some of them are the initial-rise (IR) method, curve fitting methods, Chen's half-width methods, heating rate methods and isothermal decay analysis methods. However, almost all of the developed expressions in

these methods assume the frequency factor s is temperature independent. But it has been shown that this assumption results in significant errors in the values of the trapping parameters (E, s, l).

Keating [6] has suggested that the temperature dependent frequency factor arises from the influence of the temperature dependent trapping cross section σ with $T^x(-4 \leq x \leq 0)$, the mean thermal velocity of a free carrier ν with $T^{1/2}$ and the effective density of states in the conduction band N_c with $T^{3/2}$. The effect of the temperature dependent frequency factor on the evaluated trapping parameters have been discussed earlier in detail [7-10] and they have come to the conclusion that if the temperature dependent frequency factor is not considered in the evaluation of trapping parameters there will be large errors in the evaluated trapping parameters. On the other hand, the determination of the temperature dependent frequency factor constant b from the TL glow curve is a controversial subject among investigators. Keating [6] has suggested an experimental method to estimate b by using the four quantities from the TL glow curves, namely peak temperature T_m, low and high half-intensity temperatures T_1, and T_2 and heating rate β. Fleming [11] criticizes the correctness of Keating's method [6] and claims that the constant b cannot be determined from the TL glow curve alone. However, in this study a new method, based on the theoretical and experimental analysis of TL glow curves, is proposed as a way to determine the constant b from the TL glow curve alone.

2. Theory

Keating [6] has suggested that the frequency factor s, which was assumed to be constant, may vary with temperature like T^{-b}, where $-2 \leq b \leq 2$. Thus the frequency factor s can be written as in the form of

$$s = s_0 T^b. \tag{1}$$

Following Fleming [11], the equation for the glow intensity for a first-order (l=1) TSL peak for a temperature dependent frequency factor is given by

$$I(T) = C n_0 s_0 T^b \exp\left[-\frac{E}{kT} - \frac{s_0}{\beta}\int_{T_0}^{T} T^b \exp\left(-\frac{E}{kT'}\right) dT'\right] \tag{2}$$

and for non-first order kinetics ($l \neq 1$) by

$$I(T) = C n_0 s_0 T^b \exp\left(-\frac{E}{kT}\right)\left[1 + \frac{s_0(l-1)}{\beta}\int_{T_0}^{T} T^b \exp\left(-\frac{E}{kT'}\right) dT'\right]^{-\frac{l}{l-1}}. \tag{3}$$

From the shape of curves of equations 2 and 3, a general formula to determine E was given by [7-9]:

$$E = (C_{\alpha_1} + C_{\alpha_2} b)\frac{kT_m^2}{\alpha} + (D_{\alpha_1} + D_{\alpha_2} b)2kT_m, \tag{4}$$

where α is ω, τ or δ. The symbols ω, τ and δ are defined as the full-width of glow curve at its half-height ($\omega = T_2 - T_1$), its rising side temperature half-width ($\tau = T_m - T_1$), and its falling side temperature half-width ($\delta = T_2 - T_m$), respectively.

Methods involving two or more heating rates as a mean of determining trap depth E for TL measurements have been widely used [12-13]. According to these methods, only the shape and peak temperatures are changed for temperature dependent frequency factor glow curves. All of the trapping parameters are not affected by the heating rates. Additionally, a previous study [8] reports that heating rates do not effect coefficients $C_{\alpha_1}, C_{\alpha_2}, D_{\alpha_1}$ and D_{α_2}. Therefore, if Equation (4) is again written for two different heating rates β_1 and β_2, respectively, we obtain

$$E = (C_{\alpha_1} + C_{\alpha_2} b)\frac{kT_{m_a}^2}{\alpha_a} + (D_{\alpha_1} + D_{\alpha_2} b)2kT_{m_a} \tag{5}$$

$$E = (C_{\alpha_1} + C_{\alpha_2} b)\frac{kT_{m_b}^2}{\alpha_b} + (D_{\alpha_1} + D_{\alpha_2} b)2kT_{m_b} \tag{6}$$

where α_a and α_b are the temperature differences between the peak temperatures and minimum and maximum half-intensity temperatures in the case of β_1 and β_2, respectively. From Equations (5) and (6), the b can be written as

$$b = \frac{C_{\alpha_1}\left(\frac{kT_{m_a}^2}{\alpha_a} - \frac{kT_{m_b}^2}{\alpha_b}\right) + D_{\alpha_1}(2kT_{m_a} - 2kT_{m_b})}{C_{\alpha_2}\left(\frac{kT_{m_b}^2}{\alpha_b} - \frac{kT_{m_a}^2}{\alpha_a}\right) + D_{\alpha_2}(2kT_{m_b} - 2kT_{m_a})}. \tag{7}$$

In order to determine the value of b, the values of T_{ma}, T_{mb}, α_a and α_b are taken from experimental TL glow curves. The values of the coefficients $C_{\alpha 1}, C_{\alpha 2}, D_{\alpha 1}$, and $D_{\alpha 2}$ are given in the tables of previous studies [7-9] for a given value of kinetic order l. Then the value of b is determined using Equation (7).

3. Results and Conclusions

First-order TL peaks have been numerically calculated as having trap depth E = 1.6 eV, $b = 1$, and $s_0 = 1^*10^{13}$ for two different heating rates $\beta_1 = 1^\circ C/sec$ and $\beta_2 = 5^\circ C/sec$ as illustrated in Figure 1. The evaluated values of peak, for low and high half-intensity temperatures as well as their differences α_a and α_b for $b = -1, 0, 1$ and 2 and the coefficients $C_{\alpha 1}, C_{\alpha 2}, D_{\alpha 1}$, and $D_{\alpha 2}$, are given in Table 1. It is clear in Table 1 that only the characteristic parameters T_m and α of the TL glow curves changed with heating rates. During the calculation of b, the parameters α_a and α_b in Equation (7) must be chosen from one of ω, τ or δ. In this work, ω is chosen to determine the value of b. Then, the value of b is determined by means of Equation (7) using the values in Table 1 and it is seen that the calculated and input values of b are in good agreement for every value of b.

Table 1. Characteristic parameters of computer produced first-order TL glow peaks with E = 1.6 eV and $s_0 = 1^*10^{13} s^{-1} \circ C^{-b}$

Input b		$\beta_1 = 1^\circ K/sec$				$\beta_2 = 5^\circ K/sec$			Calculated b
-1		$T_1 = 658.3$	$T_m = 694.6$	$T_2 = 721.1$		$T_1 = 696.5$	$T_m = 737.4$	$T_2 = 767.2$	-1.01
	α_a	$\tau = 36.4$	$\delta = 26.5$	$\omega = 62.8$	α_b	$\tau = 40.9$	$\delta = 29.9$	$\omega = 70.7$	
0		$T_1 = 541.9$	$T_m = 565.5$	$T_2 = 582.4$		$T_1 = 567.0$	$T_m = 592.9$	$T_2 = 611.5$	0
	α_a	$\tau = 23.6$	$\delta = 16.9$	$\omega = 40.5$	α_b	$\tau = 25.9$	$\delta = 18.6$	$\omega = 44.5$	
1		$T_1 = 463.4$	$T_m = 480.2$	$T_2 = 492.1$		$T_1 = 481.4$	$T_m = 499.5$	$T_2 = 512.4$	0.99
	α_a	$\tau = 16.8$	$\delta = 11.9$	$\omega = 28.7$	α_b	$\tau = 18.1$	$\delta = 12.9$	$\omega = 31$	
2		$T_1 = 406.6$	$T_m = 419.2$	$T_2 = 428.2$		$T_1 = 420.2$	$T_m = 433.7$	$T_2 = 443.2$	1.98
	α_a	$\tau = 12.7$	$\delta = 8.9$	$\omega = 21.6$	α_b	$\tau = 13.5$	$\delta = 9.5$	$\omega = 23$	
	$C_{\alpha 1}$	1.4600	0.9852	2.4430	$D_{\alpha 1}$	-2.1695	-0.17590	-1.30610	
	$C_{\alpha 2}$	-0.00251	-0.00024	-0.00031	$D_{\alpha 2}$	-0.90258	-0.98906	-0.97291	

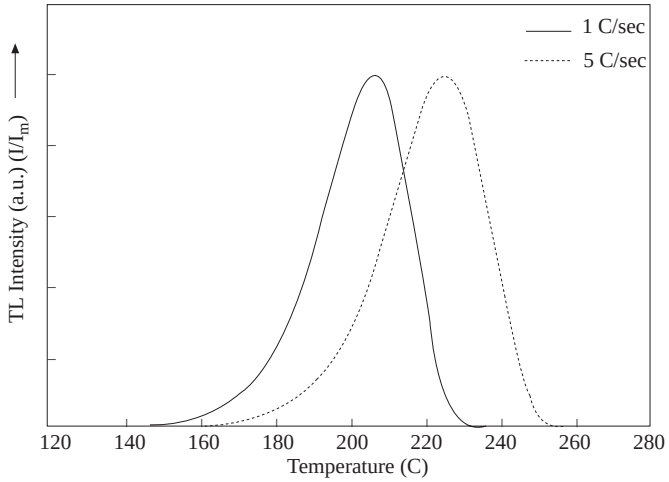

Figure 1. Computer produced first-order TL peaks with E = 1.6 eV, $b = 1$ and $s_0 = 1^*10^{13}$. a) $\beta_1 = 1Ks^{-1}$, b) $\beta_2 = 5Ks^{-1}$.

However, in the experimental measurements, the exact determination of peak, low and high half-intensity temperatures are very difficult. But, this problem has been reduced to the minimum point with the development of a new technological TL reader. Therefore, according to the proposed method, the determination of b from only the TL glow curve is possible and it gives the best result.

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