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A Study on the Correction of the Trap Depth Value for Low Temperature TL Peak of Quartz

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Abstract – One of the significant factors that should be examined when performing a thermoluminescence (TL) study related to a natural material is the detection of the trap depth. The various heating rate (VHR) method is one of the practical methods used in the calculation of the trap depth. Even though the HRs used in TL measurements do not affect the trap depth of the thermoluminescent materials, the corrected TL peak data should be used in the calculation of the trap depth. In this paper, low temperature TL glow peak of natural quartz (NQ) was recorded by using different linear HRs between 0.5 and 10 K/s from room temperature (RT) to 425 K by applying the same irradiation with the beta dose of 0.5 Gy. The trap depth of NQ sample was calculated using VHR method for both experimental and corrected TL glow peaks of NQ. The trap depth values were found to be 0.57 ± 0.03 and 0.79 ± 0.04 eV with VHR and Mott-Seitz correction methods, respectively.

Keywords – Quartz, thermoluminescence, heating rate, temperature lag, trap depth.

I. Introduction

Luminescence is the emission of light from a natural or synthesized phosphor following the initial absorption of energy from an external source of the radiation [1]. Thermoluminescence (TL) is a type of luminescence which can be observed when the phosphor is thermally stimulated [2]. As a fact of physical phenomena, a certain property of the material under study is measured as a function of the temperature in thermally stimulated processes [1]. TL research tool is extensively utilized in the fields of radiation dosimetry, dating [3] and determining the kinetic parameters (trap depth, frequency factor, and order of kinetics) of the luminescent materials. In order to evaluate the trap depth (or activation energy), various methods have been developed and applied. The various heating rate (VHR) method is one of the practical methods used in the calculation of the trap depth especially. In TL measurements, there are two undesirable conditions in the high values of the HR: temperature lag and thermal quenching.

The first of these conditions is the temperature lag effect. When the HR changes the maximum temperature (T_M) of the peak also changes: at faster HRs correspond a shift temperature towards higher values of T_M [4]. In TL readers, the temperature is measured using a thermometric device (e.g. thermocouple), therefore there might be a temperature difference between the temperature of the sample and that of the thermocouple [5]. An occurred difference in the temperature between the thermocouple and the sample is known as the temperature lag effect [6-9]. Kitis and Tuyn [10] suggested a methodology for the correction of temperature lag effect using only TL measurements based on the following equation:

$$T_j = T_i - c \cdot ln\left(\frac{\beta_i}{\beta_j}\right) \qquad (Eq.1)$$

where T_i and T_j are the TL peak maximum temperatures obtained at HRs β_i and β_j (β_j>β_i), respectively and c is a constant with the value of $\frac{T_i - T_j}{ln(\beta_i/\beta_j)}$. In the calculation of c value, T_i and T_j must be selected as the peak maximum temperature of the first two lowest HRs.

The second undesirable condition is thermal quenching in the calculation of trap depth using VHR method. Thermal quenching generates a decrease in the luminescence efficiency (η(T)) with the increasing temperature. The effect of thermal quenching on the determination of trap depth due to the luminescence efficiency may vary with temperature [11]. This issue has been discussed earlier [12-14] in cases where the thermal quenching is attributed to the well-established mechanisms recommended by Mott and Seitz and which has been recorded for a series of luminescent materials [15]. The luminescence efficiency is calculated by the following equation in the case of internal quenching.

$$\eta(T) = \frac{1}{1 + c \cdot e^{-\frac{W}{kT}}} \qquad (Eq.2)$$

where W and c are called the quenching parameters, W is thermal activation energy of quenching and c is a constant; k is Boltzmann's constant; T is the temperature in units of K.

The purposes of this study are given below:

i) The trap depth calculation of low temperature TL peak of natural quartz (NQ) using VHR method,

ii) The determination of the thermal quenching parameters,

iii) The trap depth calculation using the Mott-Seitz correction.

II. Materials, Instruments and Methods

In the present work, the powder NQ samples were used to calculate trap depth by VHR method. An automated lexsyg smart TL/OSL reader system which has an internal Hamamatsu bi-alkaline photomultiplier tube (PMT) and an internal $^{90}Sr/^{90}Y$ beta radiation source was used for the TL measurements. The dose rate, activity and maximum energy of the beta source are 0.11 Gy/s, 1.85 GBq and 2.2 MeV, respectively. A filter (IRSL, TL-565 nm: Schott-BG 39-Glass-3 mm; AHF-BrightLine HC 575/25-Interference-5 mm) was selected in front of the PMT. TL readouts were performed at the HRs between 0.5 and 10 K/s from room temperature (RT) to 425 K. Finally, the net TL intensity was obtained by subtracting the background from the initial TL data.

III. Results and Discussions

TL glow peak data of NQ samples exposed to ~ 0.5 Gy beta dose were evaluated using the HRs in the range of 0.5–10 K/s and the obtained TL glow curve is represented in Fig. 1. As seen in Fig. 1, NQ has one main low temperature TL peak at about 340 K when the possible lowest HR value (0.5 K/s) is applied. T_M shifts to higher values of temperature and its TL peak intensity decreases with increasing HR. The TL glow peaks recorded from the measurements were observed to have the temperature lag and thermal quenching characteristics as described in the introduction section.

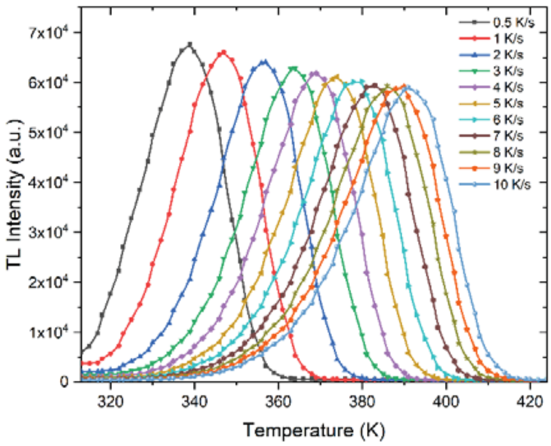

Fig. 1 TL glow peaks of natural quartz for eleven different HR values (with an irradiation of 0.5 Gy).

As seen in Fig. 2, the graph of $ln\left(T_M^2/\beta\right)$ versus $1/kT_M$ will result in a straight line with the slope equal to trap depth (E), where β is HR. This method is appropriate for any HR and supposed to be unconnected with the order of kinetics [1]. In this study, trap depth of low temperature peak of NQ by VHR method was found to be 0.57 ± 0.03 eV.

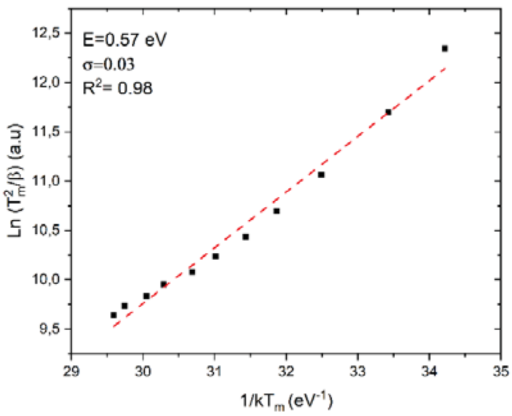

Fig. 2 Various heating rate plots of $ln\left(T_M^2/\beta\right)$ against $1/kT_M$.

The temperature lag correction is grounded on the Eq. 1 described in the introduction section and the values of T_M for the lowest HRs of 0.5 and 1 K/s were used to determine the constant c. After the constant c was calculated, the corrected values of T_M were calculated for all HRs. The uncorrected (experimental) and the corrected values of TL glow peak temperatures are shown in Fig. 3. The black solid squares and the red solid circles, for TL glow peaks, express the uncorrected values and the corrected ones found using Eq. 1, respectively. It can be easily observed that the difference between uncorrected and corrected T_M values, which defines the temperature lag correction, becomes obvious for higher HRs.

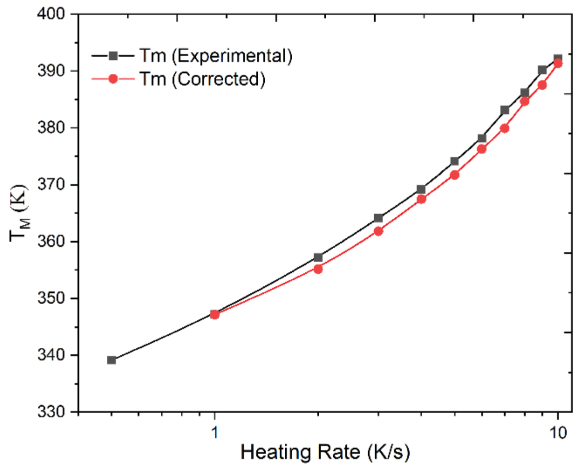

Fig. 3 T_M as a function of the HR for low temperature TL glow peak of NQ.

As it is known, trap depth value of any TL glow peak can be easily calculated as above using experimental TL data obtained from VHR measurements, but the calculated trap depth values will be most likely erroneous for the experimental TL glow peak. Therefore, the error correction is mandatory in the calculation of trap depth using experimental TL glow peak data with VHR method. In the present study, the corrected value of trap depth was calculated using thermal quenching parameters (W and c) with Mott-Seitz theory described in the introduction section. As seen in Fig. 4, in order to calculate W and c values, $ln\left(\frac{I_u}{I_q}-1\right)$ as a function of $1/kT_M$ graph is plotted, where I_u and I_q are the unquenched and quenched TL intensity for HRs of 0.5 and 1 K/s, respectively. This graph will lead to a straight line with the slope equal to W and intercept equal to ln c.

The trap depth of non-radiative transitions is found as $W = 0.43 \pm 0.05$ eV and the c parameter is calculated as 57930.5. The corrected activation energy E_c as a function of the uncorrected one E_{uc} and Mott-Seitz parameters:

$$E_c = E_{uc} + \Delta E \qquad (Eq.\ 3)$$

where

$$\Delta E = \frac{W}{1+\left[cxe^{-\frac{W}{kT}}\right]^{-1}} \qquad (Eq. 4)$$

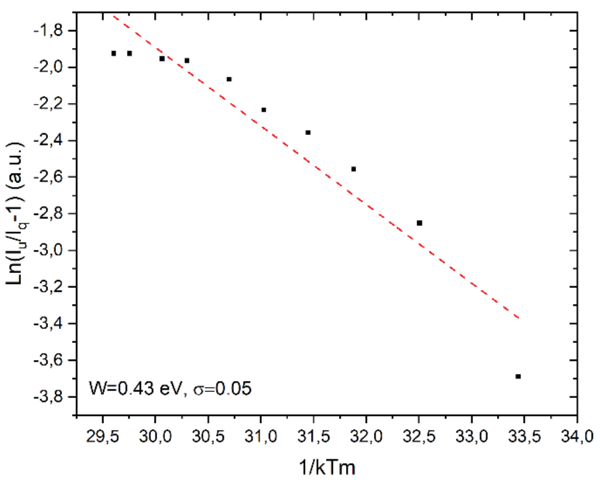

Fig. 4 The plots of $ln\left(\frac{I_u}{I_q}-1\right)$ against $1/kT_M$ for calculating W and c thermal quenching parameters.

When the correction is applied to the experimental result using the correction formulas, Eq. 3 and 4, the corrected trap depth value was obtained as $E_c = 0.79 \pm 0.04$ eV. The calculated results of the uncorrected and corrected trap depth values using VHR method and Mott-Seitz theory are shown briefly in Table 1.

Table 1. Trap depths obtained from VHR method and Mott-Seitz correction.

Method	T_M **(K)**	**E (eV)**
Various Heating Rate (VHR)	340	0.57 ± 0.03
Mott-Seitz Correction	340	0.79 ± 0.04

IV. CONCLUSION

In this study, the low temperature TL glow peaks of NQ were recorded after beta exposure of 0.5 Gy at different eleven HR values from 0.5 to 10 K/s. The results exhibit that the TL glow peak of the NQ sample has a main TL glow peak located at around 340 K when HR of 0.5 K/s was applied.

VHR measurements showed that when HR increases; TL glow peak temperature shifts to higher values of temperature and its TL peak intensity and area under the glow peak were decreasing, demonstrating the presence of temperature lag and the thermal quenching effect, respectively.

Trap depth of the NQ samples for low temperature TL peak were calculated by using VHR method. Thermal quenching parameters applying Mott-Seitz correction determined as $c = 57930.5$ and $W = 0.43 \pm 0.05$ eV. As seen in Table 1, the low temperature peak studied presents the corrected values of trap depth as $E_c = 0.79 \pm 0.04$ eV.

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