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New numerical model for thermal quenching mechanism in quartz based on two-stage thermal stimulation of thermoluminescence model

Ahmed Kadari [a,b,*], **Dahane Kadri** [a]

[a] *Department of Physics, Electronic Microscopy and Materials Sciences Laboratory, Sciences and Technology University of Oran, Algeria*
[b] *Department of Sciences of the Matter, Faculty of Science and Technology and Science of the Matter, Ibn Khaldoun University, Tiaret, Algeria*

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Abstract The effect of thermal quenching plays an important role in the thermoluminescence (TL) of quartz on which many applications of TL are based. The studies of the stability and kinetics of the 325 °C thermoluminescence peak in quartz are described by Wintle (1975), which show the occurrence of thermal quenching, the decrease in luminescence efficiency with rise in temperature. The thermal quenching of thermoluminescence in quartz was studied experimentally by several authors. The simulations work presented in the literature is based on the single-stage thermal stimulation model of thermoluminescence, in spite of that the mechanisms of this effect remain incomplete. This paper presents a new numerical model for thermal quenching in quartz, using the previously published two-stage thermal stimulation of thermoluminescence model.

1. Introduction

The thermal quenching of luminescence efficiency is an effect which is present in many thermoluminescent (TL) materials. It causes a significant decrease of the luminescence signal and disturbs the shape of the glow-peaks. Among the TL materials which exhibit thermal quenching, the most widely known and investigated are Al_2O_3:C (Akselrod et al., 1990, 1998; Kitis et al., 1994) and Quartz (Wintle, 1975; McKeever et al., 1997; Kitis et al., 2003; Petrov and Bailiff, 1996, 1997; Chitambo, 2003). Heating rate is one of the most important experimental variables, which changes the glow curve shape (Ogundare et al., 2005). In TL dosimetry, the absorbed dose and TL intensity are affected by changes in the heating rate (Betts et al., 1993; Taylor and Lilley, 1982).

Many investigations have been carried out by scientists in order to understand that how the TL glow curve changes under different heating rates (Taylor and Lilley, 1982; Nakajima,

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[*] Corresponding author at: Department of Sciences of the Matter, Faculty of Science and Technology and Science of the Matter, Ibn Khaldoun University, Tiaret, Algeria. Tel.: +213 7 75 95 56 27.
E-mail address: kadariahmed_14@yahoo.fr (A. Kadari).

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1976; Jain, 1978; Spooner and Franklin, 2002). The decrease of luminescence efficiency with temperature increase due to the increased probability of non-radiative transitions is known as thermal quenching (Curie, 1963).

The effect of thermal quenching may be observed while performing a series of TL measurements with different heating rates. Typically, with increasing heating rate, the maximum of a TL glow peak shifts to higher temperatures. At a higher temperature, the luminescence is quenched more intensely so that the whole area under TL peak decreases.

The thermal quenching efficiency versus temperature, $\eta(T)$, is given by the following equation (Petrov and Bailiff, 1996, 1997):

$$\eta(T) = \frac{1}{1 + C.\exp(-\frac{W}{kT})}, \tag{1}$$

where C and W are ‘quenching parameters’. T is the sample temperature and k is the Boltzmann constant (Akselrod and Larsen, 1998).

(Wintle, 1975), measured the thermal quenching parameters of annealed natural quartz using radioluminescence as $C = 2.8 \times 10^7$ and $W = 0.64$ eV indicating that the quenching properties are independent of the wavelength of the observed luminescence, except at 495 nm. In this study the thermal quenching parameter values of (Wintle, 1975) will be considered as reference values. As a result of many studies, a decrease in TL intensity was observed with an increase in the heating rate. This phenomenon has been explained to be due to thermal quenching, whose efficiency increases as temperature increases (Spooner and Franklin, 2002).

The thermal quenching mechanism in quartz based on time-resolved optically stimulated luminescence has been studied by Pagonis et al. (2010). The aim of the present paper is to investigate a new numerical model which described a thermal quenching in quartz, based on the previously suggested two-stage thermal stimulation of thermoluminescence model by Chen et al. (2012).

2. The proposed model

Fig. 1 shows the energy level diagram of the proposed model based on the two-stage thermal stimulation of thermoluminescence mechanism (Chen et al., 2012). The model consists of many trapping states and one kind of recombination center, with the corresponding electronic transitions taking place during excitation and heating stages.

In the model described below, $N(\mathrm{cm}^{-3})$ is the concentration of the trapping state, $n_1(\mathrm{cm}^{-3})$ is their instantaneous occupancy; $n_e(\mathrm{cm}^{-3})$ is the instantaneous occupancy of the excited state. The activation energy and the frequency factor for this transition are E_1(eV) and $s_1(\mathrm{s}^{-1})$, respectively. Once the electron is in the excited state, it can either retrap with a probability of $p(\mathrm{s}^{-1})$ or be thermally excited into the conduction band. The activation energy and the frequency factor for this transition are E_2(eV) and $s_2(\mathrm{s}^{-1})$, respectively. $n_c(\mathrm{cm}^{-3})$ are the instantaneous concentration of electrons in the conduction band. $A_n(\mathrm{cm}^3\ \mathrm{s}^{-1})$ is the retrapping probability coefficient of electrons from conduction band into the excited state, $A_m(\mathrm{cm}^3\ \mathrm{s}^{-1})$ is the recombination probability of electrons with holes in the recombination centers.

The electronic transition from the conduction band into the excited state of recombination center (located below the conduction band) is denoted by the probability A_{n2}. The direct radiative transition from the excited level into the ground electronic state of recombination center is given by the probability A_m, this recombination is assumed to produce the TL photons with an instantaneous intensity I. The probability for the competing thermally assisted process is given by a Boltzmann factor of the form $A_{\mathrm{NR}}.\exp(-W/k_BT)$ where W represents the activation energy for this process and A_{NR} a constant representing the non-radiative transition probability coefficients (s^{-1}). The dashed arrow denotes the non- radiative process into the ground state, $N_2(\mathrm{cm}^{-3})$ and $n_2(\mathrm{cm}^{-3})$ are the concentrations of electron traps and filled traps correspondingly in the excited state of the recombination center, $M(\mathrm{cm}^{-3})$ and $m(\mathrm{cm}^{-3})$ are, respectively the concentration of traps and holes in the ground electronic state of recombination center.

The simultaneous differential equations governing the process during the heating stage, shown in Fig. 1 are:

$$\frac{dn_1}{dt} = -s_1 n_1 \exp(-E_1/kT) + pn_e, \tag{2}$$

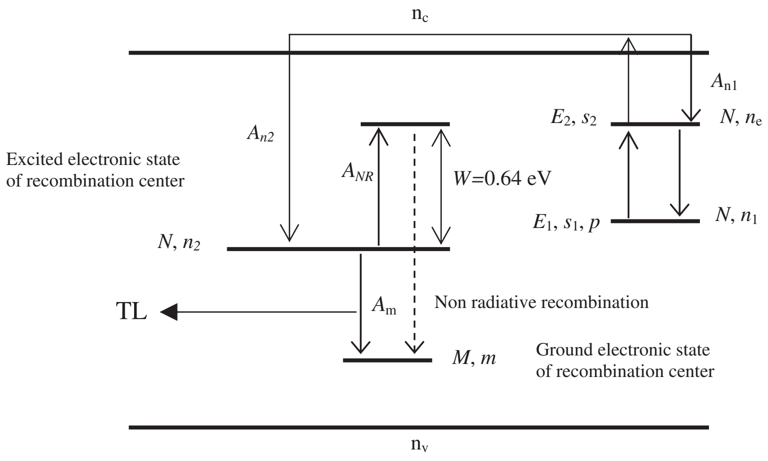

Figure 1 Schematic diagram of the thermal quenching model for quartz, using the two-stage thermal stimulation of the thermoluminescence model. The various transitions shown and the parameters used in the model are described in the text.