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Original research article

Trapping parameters determination and modeling of the thermoluminescence process in SiO_2-P_2O_5 vitroceramics doped with different Y_2O_3 concentrations

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ABSTRACT

The $xY_2O_3\cdot(60-x)P_2O_5\cdot 40SiO_2$ vitroceramic compounds exhibited excellent TL output following beta irradiation, especially when doped with high Y_2O_3 concentrations, as showed in a recent work conducted by Biró et al., 2015. In the first section of this paper, the previous recorded TL glow peaks were further analyzed and their corresponding kinetic parameters such as an order of kinetics (b), trap depth (E) and frequency factor (s) were determined using the Chen's peak shape method. In the second section, the thermoluminescence characteristics of SiO_2-P_2O_5 doped with different Y_2O_3 concentrations were simulated using the TTOR (Two traps & one recombination center) model. All calculated TL glow curves were in good agreement with the experimental results.

1. Introduction

The energy structure of crystals can be found by investigating the glow curves corresponding to different stimulations [1]. The intensities, position and shape of the glow peaks are related to the trap states responsible for the thermoluminescence phenomenon [2]. Kinetic parameters give valuable information about the TL mechanism and the trap level distribution in materials. So, it is important to know the kinetic parameters associated with different traps for each glow peak [3]. The dosimetric properties of every TL material especially depend on its trapping parameters which represent the defect centers responsible for the TL emission [4]. Investigations of radiation induced defect centers using the thermoluminescent characteristics of glass systems, polycrystalline ceramics and vitroceramics have been extensively undertaken in recent years [4–10]. Moreover, various experimental techniques such as isothermal decay analysis methods, curve fitting methods or Chen's peak shape method have been developed to determine the trapping parameters from TL glow curves [11–18].

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In a recent study, Biró et al. [19] assessed the usefulness of $xY_2O_3{\cdot}(60-x)P_2O_5{\cdot}40SiO_2$ vitroceramic system doped with xY_2O_3 at various concentrations ($0 \le x \le 30$ mol%) as luminescence dosimetric material. It was found that 20 mol% and 30 mol% Y_2O_3 doped vitroceramics exhibited bright TL signals characterized by a less complicated structure of the glow curves, linear dose response dependence, poor fading signal, low minimum detectable doses and satisfactory repeatability and homogeneity properties [19].

This paper provides a detailed kinetic study of the previously recorded thermoluminescence glow peaks of SiO_2-P_2O_5 vitroceramics doped with varying concentrations of Y_2O_3 using a refined peak fitting approach. Furthermore, the thermoluminescence properties of all investigated samples were simulated using the TTOR (Two traps & one recombination center) model.

2. Thermoluminescence properties

The samples were irradiated with 6 Gy using a ^{90}Sr-^{90}Y beta source and the TL signals were recorded at a controlled heating rate of 5 °C s^{-1} after applying thermal treatments consisting of a 10 s preheat at 150 °C for samples doped with 0–15 mol% Y_2O_3 and at 175 °C in the case of 20 and 30 mol% Y_2O_3, respectively [19]. All samples were characterized by similar main glow curves, with peak 1 and 2 centered at the temperature range from 450 K to 540 K, except the fifth sample (SiO_2-P_2O_5 (30% Y)),which only has a single TL peak at 489 K. The peaks position and the maximum TL intensity were increased by adding growing Y_2O_3 concentrations into the material. Thus, the Y_2O_3 ion doping has shown to cause significant increase in TL emissions. Actually, the major role of Y_2O_3 ions in the TL mechanism is the trap filling process that may arise through the direct transfer of electrons from the excited state to trap centers. In this study, the obtained TL glow curves were deconvoluted using the glow curve deconvolutions GCD published by Kitis et al. [14] and the results are shown in Fig. 1. Firstly, the overlapped peaks were separated into single glow peaks, and then the analysis of the obtained sets of individual glow peaks was performed using the Chen's peak shape method [13].

3. Trap parameters determination

The Chen's peak shape method is widely used for analyzing TL glow curves in order to ascertain the kinetic parameters E, s, and b considering the shape or geometrical properties of the peak. TL glow peaks corresponding to second-order kinetics are characterized by an almost symmetrical shape, whereas first-order peaks are asymmetrical. This method is useful for a broad range of energies ranging between 0.1 eV and 2.0 eV, and for values of the frequency factors between 10^5 s^{-1} and 10^{23} s^{-1}. When applying this method, the trap depth is given by the following equation:

$$E_\alpha = c_\alpha \left(\frac{kT_m^2}{\alpha}\right) - b_\alpha(2kT_m) \tag{1}$$

where α corresponds to $\tau = (T_m - T_1)$, $\delta = (T_2 - T_m)$ and $\omega = (T_2 - T_1)$.

Here, T_m is the maximum peak temperature, T_1 and T_2, respectively are the temperatures on either side of T_m, corresponding to the half intensity of the glow peak and k is the Boltzmann constant ($k = 8.6 \times 10^{-5}$ eV K^{-1}).

The values of C_α and b_α are summarized below.

$$C_\tau = 1.51 + 3.0(\mu_g - 0.42), b\tau = 1.58 + 4.2(\mu_g - 0.42)$$

$$C_\delta = 0.976 + 7.3(\mu_g - 0.42), b_\delta = 0$$

$$C_\omega = 2.52 + 10.2(\mu_g - 0.42), b_\omega = 1$$

Chen's method does not require knowledge of the kinetic order, which is found by using the symmetry factor (μ_g) described by the equation:

$$\mu_g = \frac{T_2 - T_m}{T_2 - T_1}$$

The frequency factor (s) is given by the following relationship:

$$s = \frac{\beta E}{kT_m^2} \exp\left(\frac{E}{kT_m^2}\right)\left[1 + (b-1)\frac{2kT_m}{E}\right]^{-1} \tag{2}$$

where β is the linear heating rate ($\beta = 278$ K s^{-1}).

Table 1 presents the calculated trapping parameters for the deconvoluted peaks of SiO_2-P_2O_5 vitroceramics doped with different Y_2O_3 concentrations. It can be seen that most of the peaks are characterized by second-order kinetics. The average value of the activation energy varies from 1.112 eV to 1.147 eV, which corresponds to the frequency factors ranging between 5.33×10^{11} and 4.42×10^{12} s^{-1}. The electrons may traverse through the sample lattice depending upon their energy and the lattice composition, but they are finally trapped, forming color centers. Then, the charge carriers may form excitons with energy states (point defects) in the forbidden gap of the sample. This process leads to the formation of electron and oxygen