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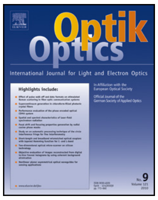

Short note

Dose dependence effect of thermoluminescence process in $TlInS_2$:Nd single crystals

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ABSTRACT

In this paper, thermoluminescence (TL) properties of $TlInS_2$:Nd single crystals were modeled using an interactive model (one trap and one kind of recombination center). The simulated work presented here was based on the experiment conducted by Delice et al. The thermoluminescence glow curve of $TlInS_2$:Nd single crystals has been characterized by one main peak at 26 K, which confirm the presence of one active electron trap level in the forbidden band of this material. The model used in this work is similar to other models cited previously in the literature. The calculated glow curve was in good agreement with the experimental one. Our numerical results show also that the thermoluminescence intensity increases with the increase of the dose rate (D). In the selected dose level range; the thermoluminescence response is linear and no saturation can be observed.

1. Introduction

Lately, ternary compounds of semiconductor materials have become a significant subject for researchers and studies on them have gain considerable momentum. Their optical, structural and electrical capabilities [1–4] show that they carry remarkable potential to be used in producing optoelectronic devices. Ternary $TlInS_2$ is a member of semiconducting materials consisted of III and VI elements in periodic table and it possesses layered structure. The ionic-covalent bonds occur between the atoms whereas the weak van der Waals bonds are created between the sequential two-dimensional layers that are perpendicular to the (001) direction. The space group of C_{2h}^{6} characterizes the crystal symmetry of $TlInS_2$, which has monoclinic structure at room temperature [5,6]. Among ternary layered crystals, $TlInS_2$ was mostly preferred material by researchers. The physical properties of $TlInS_2$ crystal were widely investigated and reported in literature [7–11].

Several experimental techniques and simulations under the light of the theoretical models were applied for different materials in literature to characterize the trapping process of defects. $TlInS_2$ single crystals were studied by using the thermally stimulated current (TSC), photoluminescence (PL) and thermoluminescence (TL) measurements. The TSC investigations achieved in 10–90 K [12] and 100–300 K [13] temperature regions revealed the existence of five trapping levels centered at energies of 12, 14 meV [12] and 400, 570 and 650 meV [13], respectively. The PL spectra detected between 500 and 850 nm and in the temperature range 11.5–100 K established the existences of one donor level at 250 meV and one acceptor level at 20 meV in the band gap [14]. Five trapping levels with thermal activation energies of 14, 19, 350, 420 and

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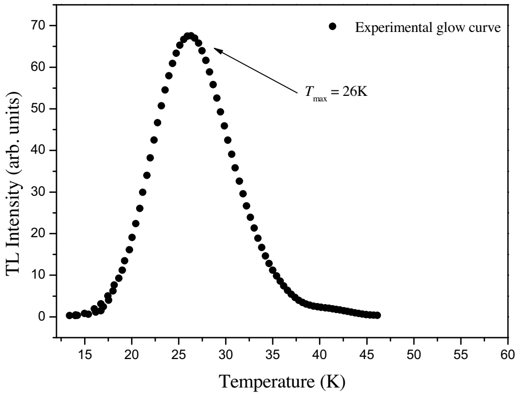

Fig. 1. Experimental TL glow curve of $TlInS_2$:Nd single crystals.

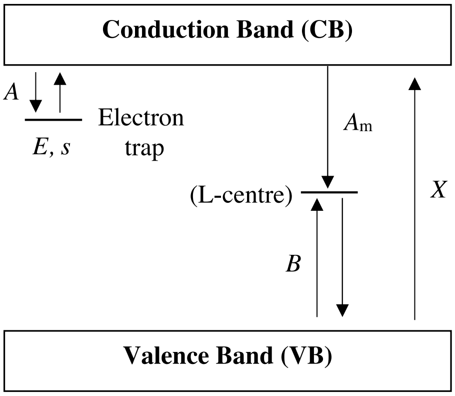

Fig. 2. Energy level diagram of the One-trap and one-recombination-center model (OTOR). The arrows indicate the possible transitions.

520 meV were revealed by achieving the TL studies on $TlInS_2$ crystal in 10–300 K temperature range [15]. TL experiments on neodymium doped $TlInS_2$ crystals carried out in the temperature range of 10–300 K were accomplished by Delice and Gasanly [16].

The TL measurements on $TlInS_2$:Nd crystals demonstrated the presence of single electron trap level in the band gap with activation energy of 14 meV. Under the light of this experimental result, TL theoretical model for this trapping level was taken into account to obtain the TL parameters. In the present paper, the thermoluminescence process of the investigated $TlInS_2$:Nd single crystals were simulated using the OTOR (one trap and one kind of recombination center) model.

2. Experimental TL glow curve

Experimental thermoluminescence (TL) glow curve of neodymium doped $TlInS_2$ crystals was recorded at the heating rate of 0.4 K s^{-1}. The obtained TL glow curve was characterized by one main peak at around 26 K (Fig. 1). This last confirm the presence of one electron trapping in the band gap of $TlInS_2$:Nd. The determination of trap parameters such as; activation energy (E), frequency factor (s) and kinetic order (b) present a major part of this study. These trap parameters have been determined previously in the recently published paper [16]. The main TL glow peak of $TlInS_2$:Nd shows the general order kinetic with $b = 1.4$ and the trap depth has been found equal to 14 meV.

2.1. The model

A physical model is a framework of ideas and concepts from which we interpret our observations and experimental results. A large number of models were widely used to study the thermoluminescence (TL) process in several luminescent materials, such as magnesium oxide (MgO) [17], double potassium fluoride (K_2YF_5) [18,19], double gadolinium fluoride (K_2GdF_5) [20], quartz [21], dolomite ($CaMg(CO_3)_2$) [22], lanthanum aluminum oxide ($LaAl_2O_3$) [23] and vitroceramics (SiO_2-P_2O_5) [24]. The thermoluminescence mechanism occurring in this ternary compounds was simulated using the OTOR model. The transitions involved in our proposed model are shown in Fig. 2.

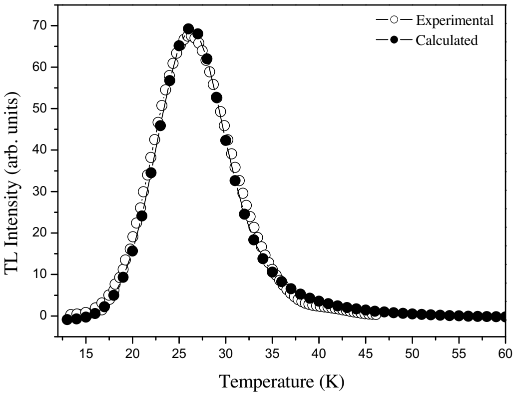

Fig. 3. Comparison between the experimental (open circle) and the calculated (black sphere) TL glow curves of $TlInS_2$ doped Nd.

During excitation stage, traffic of electrons in the electrons trap is given by the following equations (Here we assume that the transitions from electrons trap to the conduction band are not possible):

$$\frac{dn}{dt} = n_c (N - n)A, \tag{1}$$

$$\frac{dm}{dt} = n_v(M - m)B - A_m m n_c, \tag{2}$$

$$\frac{dn_v}{dt} = X - B(M - m)n_v, \tag{3}$$

$$\frac{dn_c}{dt} = \frac{dm}{dt} + \frac{dn_v}{dt} - \frac{dn}{dt}. \tag{4}$$

During the heating stage, the following differentials equations have been used:

$$\frac{dn}{dt} = n_c(N - n)A - n.s \exp\left(-\frac{E}{K_B T}\right), \tag{5}$$

$$\frac{dm}{dt} = -A_m m n_c, \tag{6}$$

$$\frac{dn_c}{dt} = \frac{dm}{dt} - \frac{dn}{dt}. \tag{7}$$

The theoretical formula of the thermoluminescence intensity is given by:

$$I(T) = n_c m.A_m. \tag{8}$$

here n is the concentration of electrons in trap, N is the corresponding concentration of electrons trap, M is the concentration of recombination centres, s is the frequency factors, E is the trap depth, K_B is the Boltzmann constant, and m is the concentration of holes in the recombination centre, n_c and n_v are the concentration of electrons and holes in the conduction and valance bands, respectively. A is the retrapping probability, B ($cm^3\,s^{-1}$) is the trapping coefficient of free holes in centre, A_m ($cm^3\,s^{-1}$) is the recombination probability and T is the temperature. X ($cm^{-3}\,s^{-1}$) is the rate of electron–hole pair production. The constant heating rate used in this work was equal to $0.4\,K\,s^{-1}$. About this work, we note that all simulations were started with empty traps and centers. Besides, the quasi-equilibrium approximation was not taken into account. The free parameters A and B, can't be extracted directly from the experimental TL glow curve, so our simulation is begins by assuming some initial guess values for these two parameters, which were set manually in such manner that the computed glow curve matched the experimental one as much as possible.

3. Results

In order to show the validity of our proposed model to reproduce the glow curve and to interpret the thermoluminescence process of $TlInS_2$ doped with neodymium ions; The system of differential equations (Eqs. (1)–(7)) were numerically solved using MATLAB code (ode23 solver). Calculated TL glow curve (black sphere) obtained after running of our proposed program and the experimentally recorded one (open circle) of $TlInS_2$:Nd are shown in Fig. 3. it can be seen from this figure, that the simulated result was in good agreement with the experimental curve recorded by Delice and Gasanly [16]. The set of trap parameters used in this modeling work are given in Table 1.

Table 1
Trap parameters of the TL peaks of $TlInS_2$:Nd used for running our proposed model.

Levels	Parameters				
	N_i (cm^{-3})	E_i	s_i (s^{-1})	A_i ($cm^3\,s^{-1}$)	B_i ($cm^3\,s^{-1}$)
1 (26 K)	4.5×10^4	14.5 meV	9.99×10^2	4.0×10^{-8}	0
L- centre.	7.0×10^7	1.0 eV	1.0×10^{10}	1.0×10^{-5}	5.0×10^{-4}

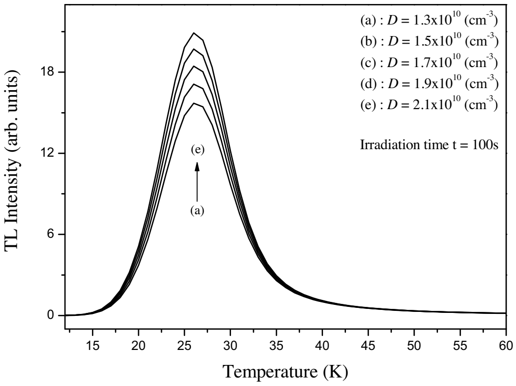

Fig. 4. Simulated TL glow curves after different dose irradiations.

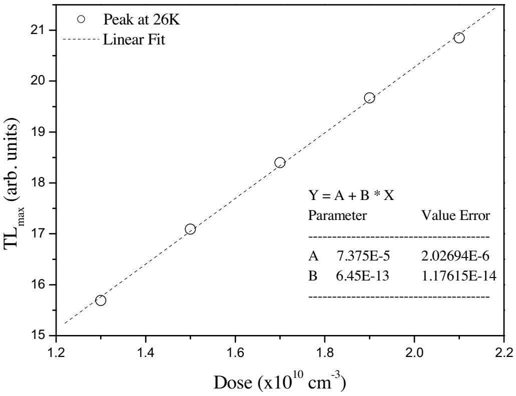

Fig. 5. Simulated dose dependence of the maximum TL intensity.

4. Dose rate dependence of TL signal

The evolution of the thermoluminescence curves as a function of the irradiated dose for the selected dose range from 1.3×10^{10} to $2.1\times10^{10}\,cm^{-3}$ is shows in Fig. 4. It was observed that the TL intensity increases with the increasing of the excitation dose rate. According to the TL theory, if the length of excitation is t_D(s), the total concentration of produced electron-hole pair is equal $X.t_D$ (cm^{-3}), which is proportional to the imparted dose. We also know that the dose dependence on the thermoluminescence glow curve gives information about the trapping process of trapped charge carriers. Our numerical results obtained in this work showed that the increase of the dose rate was not affecting the peak positions. In the case of second order kinetics, the peak positions are slightly shifts to lower temperatures [25]. This fact supported the result of experimental observation showing that the general order kinetics dominates the trapping process. Fig. 5 presents the simulated dose dependence of the maximum TL intensity. For these selected doses the TL response was found to be linear and no saturation can be observed.

5. Conclusion

In this work, thermoluminescence (TL) properties of $TlInS_2$:Nd single crystal were modeled using an interactive model (one trap and one kind of recombination centre). The experimental thermoluminescence glow curve studied in this work was conducted by Delice et al. [16]; this curve was recorded between 10 and 300 K at the heating rate of 0.4 K s^{-1}. The appear of one TL glow peak in the thermoluminescence spectrum confirm the existence of one electrons trap in the forbidden band of $TlInS_2$

doped with neodymium (Nd) ions. In order to get a best fit of the experimental glow curve, different sets of parameters were chosen to running our proposed model. Calculated TL glow curve was in good agreement with the experimental one, thus indicating the reliability of the selected trap parameters. In the selected dose level range from 1.3×10^{10} to 2.1×10^{10} cm^{-3}; the TL response was found to be linear and no saturation can be observed.

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