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Modelling of charge carriers' transport and trapping phenomena in one-dimensional structures during thermal stimulation

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Abstract

A simple model for studying charge carriers' trapping and recombination kinetics in one-dimensional insulating solids is considered. Numerical calculations are performed for linearly varying temperature that corresponds to thermally stimulated conductivity (TSC) and thermoluminescence (TL) phenomena. The influence of an external electric field on TSC and TL curves is studied. Considering a simple mono-energetic system with no external field applied one could notice two distinct peaks. The low-temperature peak corresponds to the nearest-neighbour recombination of charge carriers. The high-temperature one relates to the displacement of charge carriers along the one-dimensional structure. It is shown that low electric field changes height and position of the displacement peak. Strong electric field distorts the whole measured curve and it merges the two peaks into a single one.

Keywords: Trapping; Recombination; Thermally stimulated conductivity (TSC); Thermoluminescence (TL); Charge transport modelling; Monte Carlo simulation

1. Introduction

Electrical properties of insulating materials are determined chiefly by energy and spatial distribution of charge carriers' traps. These states located within energy gap of the solid are studied by a variety of methods. Many of them are based on the observation of thermally stimulated relaxation (TSR) phenomena. Typical examples

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are thermally stimulated conductivity (TSC) and thermoluminescence (TL). During the initial stage of these processes a sample is excited in any way—e.g., by high-energy radiation. Then, increasing temperature, one releases charge carriers' from traps. The free carriers may be recaptured by empty traps or may recombine with opposite charge carriers. Measuring conductivity of the sample or luminescence one calls the processes TSC or TL, respectively. Theoretical description of these non-equilibrium phenomena usually assumes uniform distribution of traps (the simple model [1]). Another extreme case is the model of localised transitions by Halperin and Braner [2] regarding hole–electron pairs trapped close to each other. Only for the two cases, it was possible to formulate analytical differential equations describing charge carriers' kinetics. Other cases require numerical calculations based on the Monte Carlo technique [3,4].

2. The model

When a solid is subjected to a high-energy ionizing radiation, which is typical for dosimetric applications of TL, traps and recombination centres are populated along tracks. This way, each track represents a one-dimensional (or quasi one-dimensional) structure. In such a system, spatial and energy distribution of traps could be quite complex [5]. However, to study some basic features one could consider a very simple model shown in Fig. 1 (the fixed-distance model (FD)). It is assumed that the ionising particle produces series of hole–electron pairs trapped close to each other along a track. Basic transitions of charge carriers are given by the following formulas in the form of probability densities per unit time for a single carrier:

$$D_i = v_i \exp\left(\frac{-E_i}{kT}\right), \tag{1}$$

$$T_i = A_i(N_i - n_i), \tag{2}$$

$$R_s = B_s m_s. \tag{3}$$

Detrapping (D_i) describes the escape probability of a carrier from the ith discrete trap level to the conduction band, trapping (T_i) and recombination (R_s) describe the

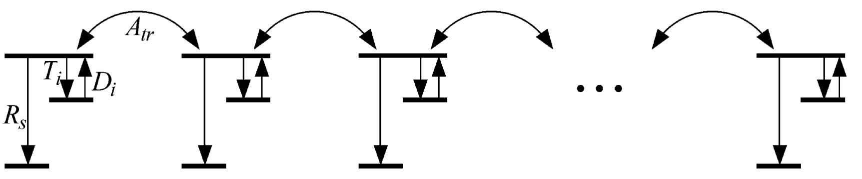

Fig. 1. One-dimensional model for TSC/TL kinetics. T_i: trapping, D_i: detrapping, R_s: recombination, A_{tr}: transition rate.

probabilities of capturing a carrier from the conduction band to the ith trap level and the sth recombination centre, respectively. E_i and ν_i denote the activation energies and frequency factors respectively; N_i, n_i, and m_s denote the concentrations of trap states, electrons trapped in 'active' traps and holes trapped in recombination centres. Because there is only one adjacent recombination centre and one free trap, the last two probabilities (2), (3) are constant (or simply $=0$ when the trap is occupied). As the simplest, mono-energetic case will be considered here, the subscripts i and s will be omitted. Additionally, electrons in excited states can move to neighbouring pairs. The transition probability A_{tr} is given by

$$A_{tr} = \nu_{tr} \exp\left(\frac{-E_{tr}}{kT}\right), \tag{4}$$

where E_{tr} represents height of potential barrier between two adjacent states. In general, the coefficient ν_{tr} could depend on the distance between trap levels. Details of the Monte Carlo algorithms were described in some earlier papers [3,4]. Radiation-induced conductivities were studied also by Arkhipov et al. [6] and others, however, their calculations relate to disordered solids within the framework of the multiple-trapping model.

3. Results

The system under study consists of long chains having 250 localised hole–electron pairs. To avoid difficulties with too short tracks periodic boundary conditions were applied. For the sake of simplicity, it was assumed in all calculations that 'active' traps have the same activation energy $E = 0.9\,\text{eV}$ and the frequency factor is $\nu = 10^{10}\,\text{s}^{-1}$, also the recombination centres have the same parameters. Considering the simplest case with no external electric field applied one could notice additional high-temperature peak on TL curves (Fig. 2(a)). External electric field increases and shifts this peak (Fig. 2(b)). The peak is due to displacement of charge carriers that avoided nearest-neighbour recombination by escaping from its native electron–hole system. The carriers recombine in another place occupying a different recombination centre. Therefore, residual charge carriers have to look for a free recombination centre along the track [7]. Luminescence intensity J_{TL} is defined as follows:

$$J_{TL} \propto \frac{dm}{dt}. \tag{5}$$

To calculate charge current it is necessary to apply an external electric field. In Fig. 3 we have two diagrams showing various quantities calculated for this case. Looking at the figures (Fig. 3(a) and (b)) it is easy to note that TSC current can be expressed by

$$J_{TSC} \propto A_{tr} n_e, \tag{6}$$

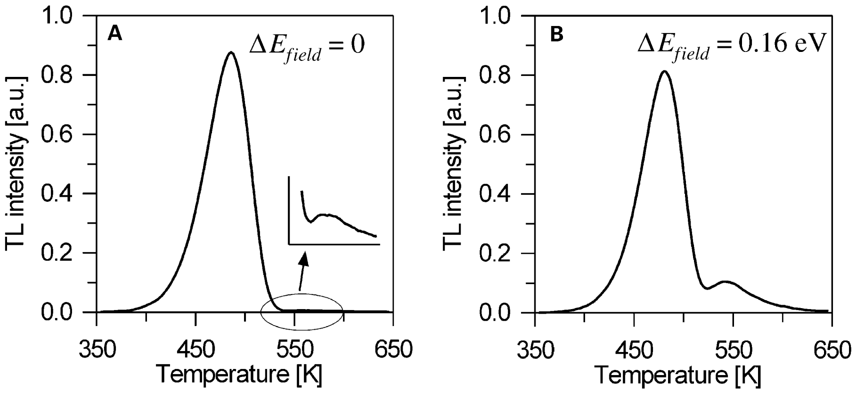

Fig. 2. TL curves calculated in the framework of the fixed distance model (Fig. 1) with thermally activated transition rate $E_{tr} = 0.8\,\text{eV}$, $\nu_{tr} = 10^9\,\text{s}^{-1}$. Trap parameters: $E = 0.9\,\text{eV}$, $\nu = 10^{10}\,\text{s}^{-1}$, retrapping coefficient $r = 100$. Diagrams calculated for the external electric field: (A) $\Delta E_{\text{field}} = 0$, (B) $\Delta E_{\text{field}} = 0.16\,\text{eV}$.

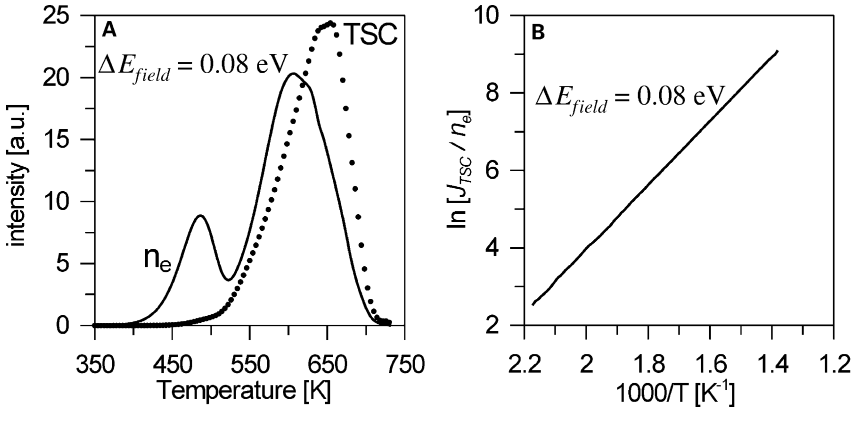

Fig. 3. (A) J_{TSC}, n_e and (B) $\ln(J_{\text{TSC}}/n_e)$ curves calculated for external electric field: $\Delta E_{\text{field}} = 0.08\,\text{eV}$. Transition rate and trap parameters are the same as in Fig. 2.

where n_e stands for the concentration of carriers in the excited states, and A_{tr} is defined by Eq. (4). The relation (6) allows calculating TSC also for the limiting case of no (or very low) external field applied.

Fig. 4 illustrates the influence of the electric field on TL curves. The strength of the field is characterised by the traps' potential lowering ΔE_{field}. For low electric fields (Fig. 4(A)), only the displacement peak changes its height and position. In a more intense field (Fig. 4 (B)), the two peaks merge into a single one. Its shape depends on the field strength.

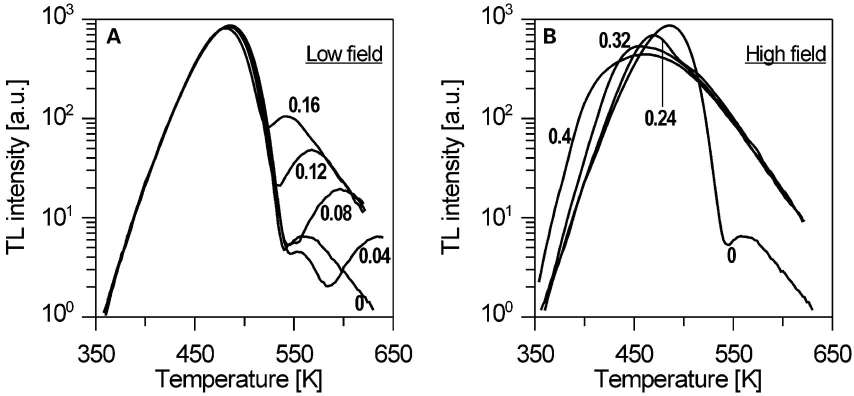

Fig. 4. J_{TL} curves calculated for various values of the external electric field: ΔE_{field} shown on the diagrams. Transition rate and trap parameters are the same as in Fig. 2. The 'zero-field curve' is shown on two diagrams for reference.

4. Conclusions

Thermally stimulated relaxation phenomena in non-homogeneous systems are complex due to many unusual properties that cannot be expressed in terms of analytical theory. Consequently, they are difficult to analyse. In this paper, a simple one-dimensional system that is likely to occur in solids, e.g., after irradiation by high-energy ionizing particles was examined. It was shown that TL and TSC curves are sensitive on the external electric field applied to the sample. Particularly, the displacement peak changes its height and position according to the external field strength. For low fields the peak grows and initially moves to higher temperatures. Then it moves backward and merges with the main peak corresponding to the nearest-neighbour recombination of carriers (Fig. 4). These features may help in the analysis of thermally stimulated data to identify the displacement peak.

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