Trapping and Recombination Properties Due to Trap Clustering

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Abstract. — Nonequilibrium charge carriers' trapping and recombination processes in semiconductors and insulators are studied by means of the Monte Carlo method The effect of trap clustering on trapping and recombination kinetics is considered. It is shown that such non homogeneous distribution of traps may significantly change some physical properties of a solid The phenomena are analysed under various conditions The influence of the temperature, the heating program and external electric field is studied The calculations are performed for various trap parameters and various types of correlations between traps. Comparing isothermal and non isothermal spectra one can conclude that temperature dependent phenomena - such as thermoluminescence - are more sensitive to trap clustering than their isothermal counterparts - *e g* isothermal phosphorescence decay

1. Introduction

Thermally stimulated relaxation phenomena are one of the basic tools to study charge carrier's kinetics in semiconductors and insulators. Theoretical description of Thermally Stimulated Conductivity (TSC) and thermoluminescence (TL) is based on traps' idea [1, 2]. The excitation (usually UV light) at appropriately low temperature fills traps with carriers. During heating with a constant rate β the probability of detrapping increases. Charge carriers released from traps to the conduction band give rise to the conductivity and, recombining, to the luminescence of the system. Keeping the sample at a constant temperature allows information about isothermal current decay (ICD) and phosphorescence decay method respectively

Recently, it was shown [3–5] that the classical model which assumes random distribution of traps and recombination centres may be not appropriate for systems with traps and recombination centres that are spatially correlated. The formation of trap clusters instead of randomly distributed defects may significantly change the kinetics of trapping and recombination processes, influencing electrical and optical properties of a solid In some, specific cases spatial correlation may produce an additional "false" TL peak [5]. First suggestions on the influence of spatial correlation on TSC and TL kinetics were published by Fields and Moran [6] and Fain and Monnin [7]. However, they have not been able to formulate any analytical theory for the description of the phenomena. Therefore, as long as such a lack prevails, it is important to study properties of TSC, TL, ICD and phosphorescence by means of numerical simulation.

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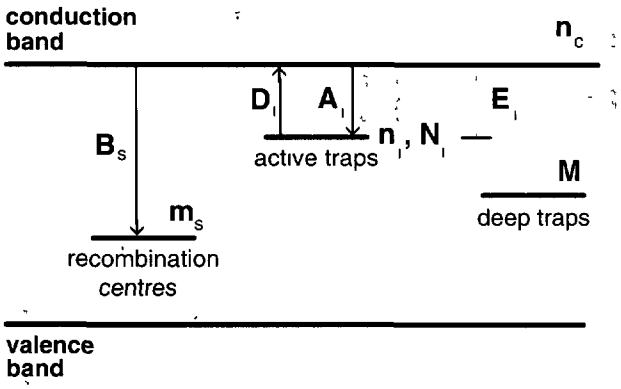

Fig. 1. — The classical band model commonly used for the explanation of thermally stimulated relaxation phenomena Allowed transitions are described by the respective probability densities. trapping (A_i), recombination (B_s) and detrapping (D_i)

2. The Monte Carlo Calculations

2.1. THE MODEL. — The energy diagram used for the calculations is presented in Figure 1. We assume that the system consists (in the considered temperature range) of a set of p discrete trap levels (here we assume electron traps), a set of k recombination centres occupied by immobilised holes and a set of deep electron traps (thermally disconnected traps). The following transitions are allowed: detrapping of a carrier to the conduction band D_i, trapping T_i from the conduction band to a given trap, and recombination R_s of a carrier from the conduction band directly to recombination centre. These can be described by the respective probabilities

$$D_i = \nu_i \exp\left(\frac{-E_i}{kT}\right) \quad (1)$$

$$T_i = A_i(N_i - n_i) \quad (2)$$

$$R_s = B_s m_s \quad (3)$$

where E_i is the energy depth of the $i-$th trap level characterised by the frequency factor ν_i, n_i stands for the concentration of trapped electrons, N_i is the total number of trapping states in this level, A_i and B_s are the trapping and recombination probabilities, respectively, m_s stands for the concentration of holes trapped in recombination centres. Let us consider M the concentration of electrons in the thermally disconnected traps, *i.e.* traps having higher activation energies. For the considered temperature range the rate of detrapping of charge carriers from these levels is very low and can be neglected. The role of these three kinds of trap levels in thermally activated processes was analysed in detail by Kelly *et al.* [8]. The concentrations of trapped electrons and trapped holes obey the following neutrality condition.

$$\sum_{s=1}^{k} m_s = \sum_{i=1}^{p} n_i + n_c = M. \quad (4)$$

We assume that the solid consists of a number of groups (clusters) having the same configuration of energy levels (Fig. 1) and separated by a distance and/or energy barriers. In the limiting case, when the transition probability of a carrier between two neighbouring groups is

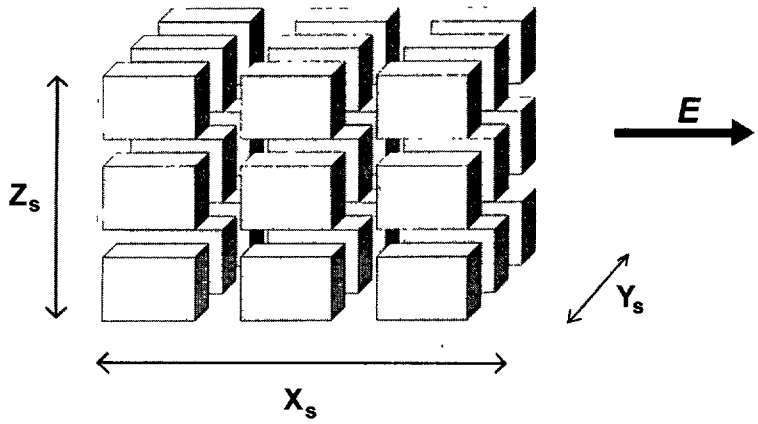

Fig. 2 — The cubic network having 10^4 cells with periodic boundary conditions. The transitions are allowed only to a nearest neighbour cell External electric field is applied along X axis

considerably smaller than recombination probability, each group can be considered, approximately, as a separate system. In order to perform each step of the Monte Carlo simulation, the times of each allowed transition were numerically generated for all carriers in the system. The times can be determined from the following integral equation.

$$\int_0^{t_i} \lambda(t')\mathrm{d}t' = -\ln(\alpha_i) \tag{5}$$

where α_i is a homogeneous normalised random variable from the interval [0, 1] and λ denotes the probability of allowed transitions, that is D_i, T_i, or R_s. At constant temperature equation (4) has a simple analytical solution, but in non isothermal cases, for $\lambda(t) = D_i(t)$ the equation has to be solved numerically. To perform Monte Carlo calculations one has to deal with absolute number of carriers instead of concentrations. The relation between macroscopic parameters appearing in equations (1-4) and the quantities used in the Monte Carlo simulation are the following:

$$\begin{cases} \bar{n}_i,\ \bar{n}_c,\ \bar{m}_s,\ \bar{N}_i,\ \bar{M} \to \chi n_i,\ \chi n_c,\ \chi m_s,\ \chi N_i,\ \chi M \\ \bar{A}_i,\ \bar{B}_i \to A_i/\chi,\ B_i/\chi \end{cases} \tag{6}$$

Here $\bar{N}_i$, $\bar{n}_i$ and $\bar{m}_s$ have the meaning of the absolute number of traps, trapped carriers and recombination centres in each group respectively and χ stands for a constant having dimension of a volume. The method of calculation was described in our previous paper [3].

2.2. TRANSPORT. — When transitions of carriers between neighbouring clusters could not be neglected the whole system (*i.e.* all groups of traps) has to be considered simultaneously. It has to be done, *e.g.* while considering the effect of an external electric field on trapping and recombination kinetics. To deal with this problem we used a cubic network of cells with periodic boundary conditions (see Fig. 2). Along with the three types of allowed transitions (1−3) a carrier in the conduction band has a chance to jump over the energy barrier to an adjacent group. The transition probability has the same form as of equation (1).

2.3. INITIAL FILLING OF TRAPS. — To perform Monte Carlo simulation for full initial filling of traps the calculations were repeated for each group with the same initial conditions.

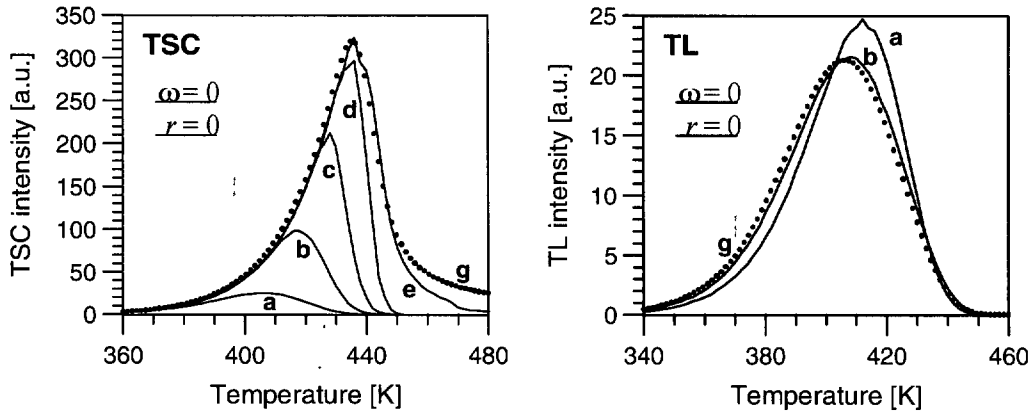

Fig. 3. — The dependence of the total number of carriers in the conduction band n_c (TSC), and the derivative $(-dm/dt)$ (TL) on the $\bar{n}_0$ absolute number of initially trapped carriers in a single separate group, during heating of the solid with a constant rate β. For the two diagrams curves (a) correspond to $\bar{n}_0 = 1$, (b) $\bar{n}_0 = 10$, (c) $\bar{n}_0 = 10^2$, (d) $\bar{n}_0 = 10^3$ and (e) $\bar{n}_0 = 10^4$. The total number of carriers in the simulation (*i.e* population of all groups) is 10^6. The case (g) corresponds to $\bar{n}_0 = \infty$.

Nevertheless, to calculate TSC and TL spectra for a system containing traps that are initially not saturated with carriers, first one has to calculate the distribution of charge carriers in the system - *i.e.* population of all groups. The process of filling the traps can be easily simulated using Monte Carlo technique [9]. The results of the preliminary Monte Carlo simulations are the input data for the main simulation program.

3. Results and Discussion

The Monte Carlo algorithm may be applied to a system consisting of any number of discrete trap levels as well as an arbitrary number of recombination centres. Nevertheless, for the sake of clarity, the calculations were performed for only one kind of traps and one type of recombination centres. Hence, instead of using notation n_i, N_i, A_i, B_s, m_s we will simplify this to n, N, A, B and m.

All the spectra were calculated for a solid having trap levels characterised by the energy depth $E = 0.9$ eV and the frequency factor $\nu = 10^{10}$ s^{-1}. Various types of spatial correlation were taken into account. They are characterised by the absolute number of carriers in a single separate group $\bar{n}_0$. During the simulation two quantities were calculated: $(-dm/dt)$, that is proportional to the luminescence of the system, an n_c - the total concentration of electrons in the conduction band. Isothermal and non isothermal cases were studied. Previously, it was found that spatial correlation affects TL and TSC spectra especially in the case of low concentrations of thermally disconnected traps ($\omega \equiv M/N \ll 1$) and high values of the retrapping coefficient $r \equiv A/B \gg 1$ [4]. Nevertheless its influence is still pronounced even for $r = 0$ (see Fig. 3). We tried to study isothermal luminescence characteristics around TL maximum. For the same case $r = 0$ almost no differences were observed between curves simulated for different population of traps in one cluster over the temperature range 350–450 K. Only since 500 K a slight difference may be observed in the final part of the curve (see Fig. 4). These curves were calculated for $\omega = 0$. However, for slightly higher concentrations of deep traps $\omega > 0.5$ no differences could be noticed. The differences in phosphorescence decay curves may

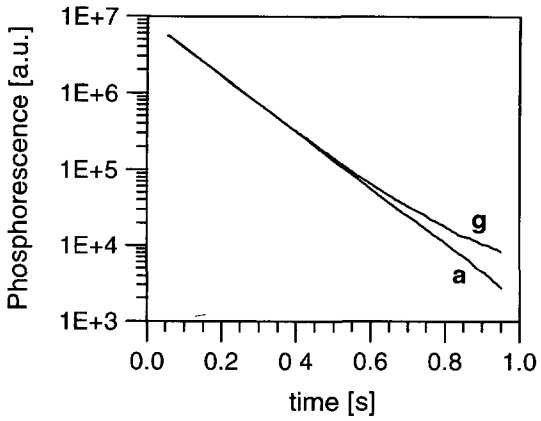

Fig. 4 — Phosphorescence decay calculated for $\omega = 0$ and $r = 0$. Curve (a) corresponds to $\bar{n}_0 = 1$ carrier trapped in a single separate group, curve (g) corresponds to $\bar{n}_0 = \infty$ (no correlated case). For $\bar{n}_0 > 10$ all curves coincide with (g)

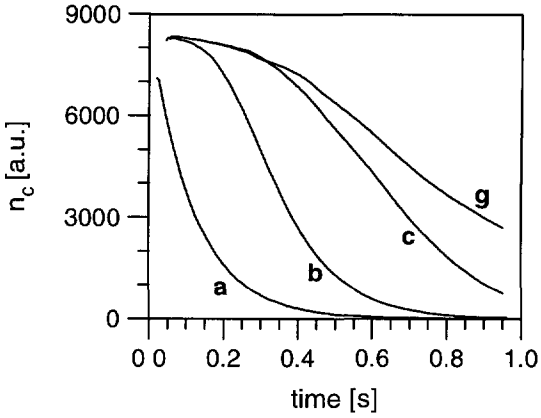

Fig. 5 — The dependence of the total population of carriers in the conduction band n_c on the absolute number of initially trapped carriers $\bar{n}_0$ in a single separate group, during isothermal decay. Trap parameters are the same as for Figure 4 For curve labelling see Figure 3

be easily observed for high values of the retrapping coefficient, but still it does not depend on the temperature of the measurement. All the differences are negligible for large clusters with the number of traps $\bar{n}_0 > 10$.

Similar calculations were performed for ICD. Unlike the phosphorescence curves ICD is very sensitive on spatial correlation of traps. This effect does not depend on the temperature and on the retrapping coefficient. Typical dependence of n_c curves on spatial correlation is shown on Figure 5. The calculations were performed for the same set of parameters as in the Figure 4. Figure 6 shows the effect of potential barrier height on the shape of TL. The calculations were performed using the cubic network of cells with periodic boundary conditions (Fig. 2). By lowering the barrier (*e.g.* by a strong electric field) one diminishes the effective separation of clusters in a solid. As a result the TL kinetics becomes "classical". Comparing isothermal

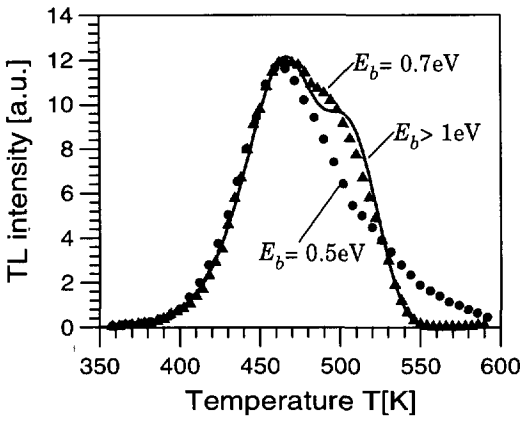

Fig. 6 — The dependence of TL spectra on the height of potential barrier E_b. The other parameters used in Monte Carlo simulation: $\bar{n}_0 = 2$, $\bar{N} = 2$, $\omega = 0$, $B = 10^{-11}$ cm^3 s^{-1}, $r = 10^2$.

and non isothermal spectra one can see that thermally stimulated relaxation spectra are more sensitive on trap clustering then their isothermal counterparts. It is particularly visible in the case of TL and phosphorescence decay.

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