ВІСНИК ЛЬВІВ. УН-ТУ VISNYK LVIV UNIV.
Серія фіз. 2009. Вип. 43. С. 143–149 Ser. Physics. 2009. Is. 43. P. 143–149

PACS number(s): 78.60.Kn

NUMERIAL VERIFICATION OF CERTAIN SCALING PROPERTY RELATING TO THERMOLUMINESCENCE PEAKS

J. Orzechowski[1], A. Mandowski[2]

[1]Stanislaw Staszic High School
ul. Szkolna 12, 27-200 Starachowice, POLAND
[2]Institute of Physics, Jan Długosz University
Armii Krajowej 13/15, 42-200 Czestochowa, POLAND
e-mail: a.mandowski@ajd.czest.pl

The phenomenon of thermoluminescence (TL) is described in terms of complex kinetic models. However, it can be shown, that TL curves exhibit several interesting scaling and invariance properties. One of them relates to the dependence of the shape of TL curves on heating rate. We suggest the conservation of a simple integral defining a part of TL peak area with respect to variable heating rate. The hypothesis is verified numerically for various parameters of traps and recombination centres.

Key words: thermoluminescence, dielectrics, traps, recombination.

The simple trap model (STM) is considered as the basic theoretical model for analyzing thermoluminescence (TL) and related phenomena. The model assumes spatially uniform distribution of separate traps and recombination centres (RCs). Charge carrier transitions taking place during heating occur via conduction band after thermal release. The kinetics of trapping and recombination is governed by the following set of differential equations [1]:

$$-\dot{n}_i = n_i \nu_i \exp\left(\frac{-E_i}{kT}\right) - n_c A_i (N_i - n_i), \qquad i=1..p, \tag{1a}$$

$$-\dot{m}_s = B_s m_s n_c, \qquad s=1..k, \tag{1b}$$

$$\sum_{s=1}^{k} m_s = \sum_{i=1}^{p} n_i + n_c + M, \tag{1c}$$

where N_i, n_i, and m_s denote the concentrations of trap states, electrons trapped in 'active' traps and holes trapped in recombination centres, respectively. M stands for the number of electrons in the thermally disconnected traps (deep traps), i.e. traps that are not emptied during the experiment. A_i and B_s stand for the trapping and recombination probabilities, respectively, and ν is the frequency factor. Luminescence intensity is proportional to $(-\dot{m})$, i.e.

$$J = -\frac{dm}{dt}. \tag{2}$$

TL spectrum consists usually of a series of peaks attributed to different trap levels of the material. Typical TL experiment is performed with linear heating rate scheme, i.e. the temperature $T = T_0 + \beta t$, where T_0 is the initial temperature, t denotes time and β is the heating rate.

The basic set of equations (1) has no analytical solutions in general case. However, some intriguing features may be observed while considering TL curves for various parameters. The simplest experimentally controllable parameter is the heating rate β. For higher heating rates TL peak shifts toward higher temperatures. Typical example of this kind is presented in fig. 1.

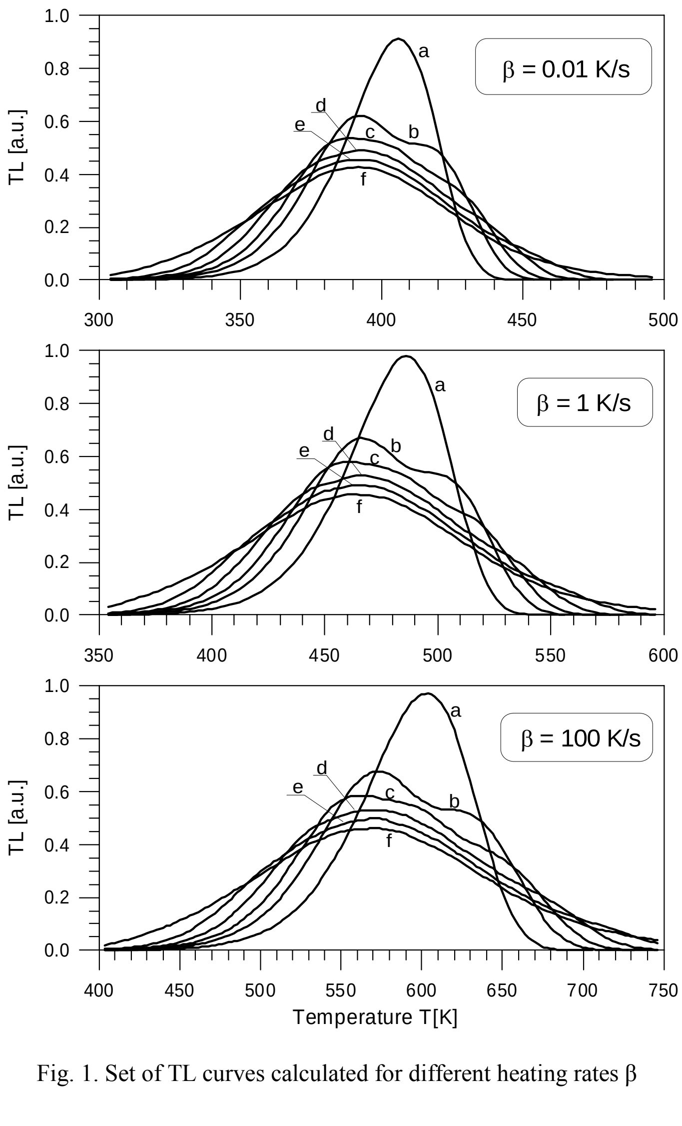

Fig. 1. Set of TL curves calculated for different heating rates β

The set of TL curves was calculated for a complex trap cluster system. The heating rates were varied over four orders of magnitude (from β=10^{-2} to β=10^{2} K/s) and the peak maximum shifts about 200 K, however its shape seems to be unchanged. This behaviour suggests the existence of a scaling property which origin is currently not known. To study these geometric features we considered the following integral:

$$S_{\varepsilon,\beta} = \int_{t_\varepsilon^{(1)}}^{t_\varepsilon^{(2)}} J(\beta,t)dt = \frac{1}{\beta}\int_{T_\varepsilon^{(1)}}^{T_\varepsilon^{(2)}} J(\beta,T)dT \,, \tag{3}$$

where $0<\varepsilon<1$ and $t_\varepsilon^{(1)}, t_\varepsilon^{(2)}, T_\varepsilon^{(1)}, T_\varepsilon^{(2)}$ denote positions on horizontal axis, on both sides of the TL peak where the intensity falls down to ε-*th* part of the maximum intensity, i.e.:

$$J\left(\beta,t_\varepsilon^{(1)}\right) = J\left(\beta,t_\varepsilon^{(2)}\right) = \varepsilon J_{\max}\,, \tag{4}$$

$$J\left(\beta,T_\varepsilon^{(1)}\right) = J\left(\beta,T_\varepsilon^{(2)}\right) = \varepsilon J_{\max}\,. \tag{5}$$

We can suppose that when the scaling is proportional, the integral (3) should not depend on the heating rate β. To check this hypothesis we performed a series of numerical calculations. The basic set of equations (1) was solved using numerical procedures for stiff differential equations. Then, the position of TL peak maximum $\left(T_{\max}, J_{\max}\right)$ was determined. Then, for a given parameter ε ($0<\varepsilon<1$), two points $T_\varepsilon^{(1)}$ and $T_\varepsilon^{(2)}$ (or $t_\varepsilon^{(1)}$ and $t_\varepsilon^{(2)}$) were found according to eqs. (4) and (5). Finally, the integral (3) between the two points was calculated. Results are shown in fig. 2.

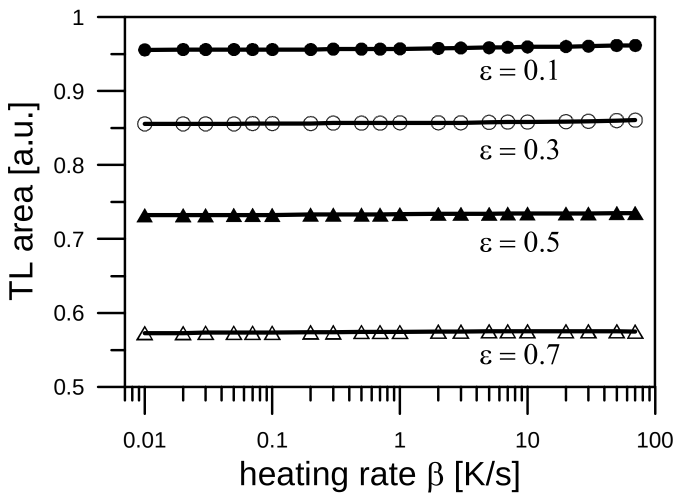

Fig. 2. Relative area under TL curve calculated for different heating rates β and various ε according to the eq. (3). The calculations were performed for the following parameters: $E = 1\,\text{eV}$, $B = 10^{12}\ \text{cm}^3\text{s}^{-1}$, $M = 0$, $N = 2\cdot10^{15}\ \text{cm}^{-3}$, $\nu = 10^{10}\ \text{s}^{-1}$ and $r \equiv A/B = 0{,}01$

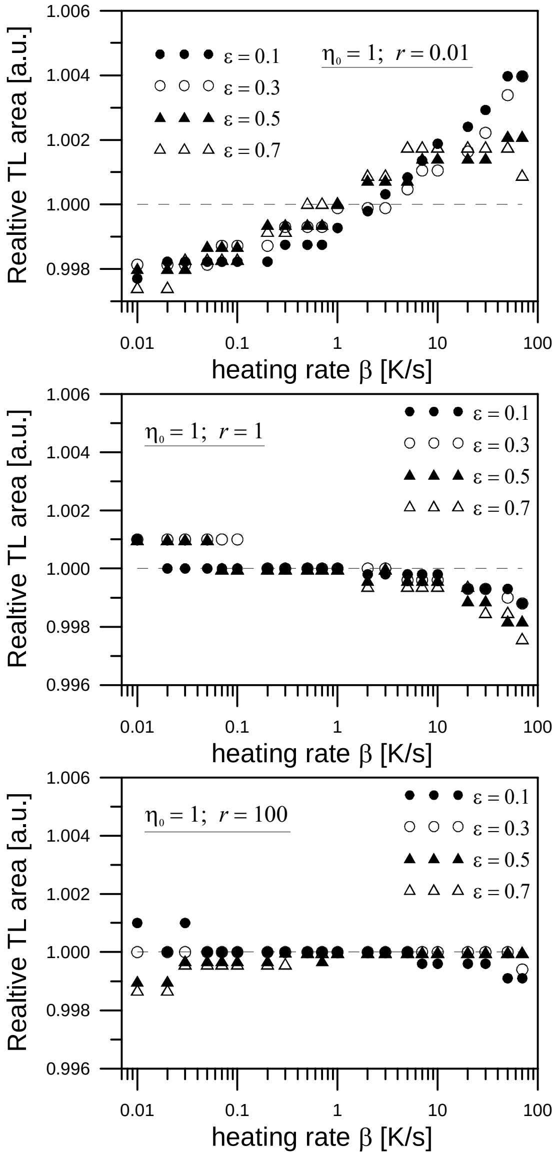

Fig. 3. Relative area under TL curve calculated for different heating rates β and various ε according to the eq. (3). Results for full initial filling of traps $\eta_0 = 1$ and various retrapping coefficients. Other parameters the same as for fig. 2

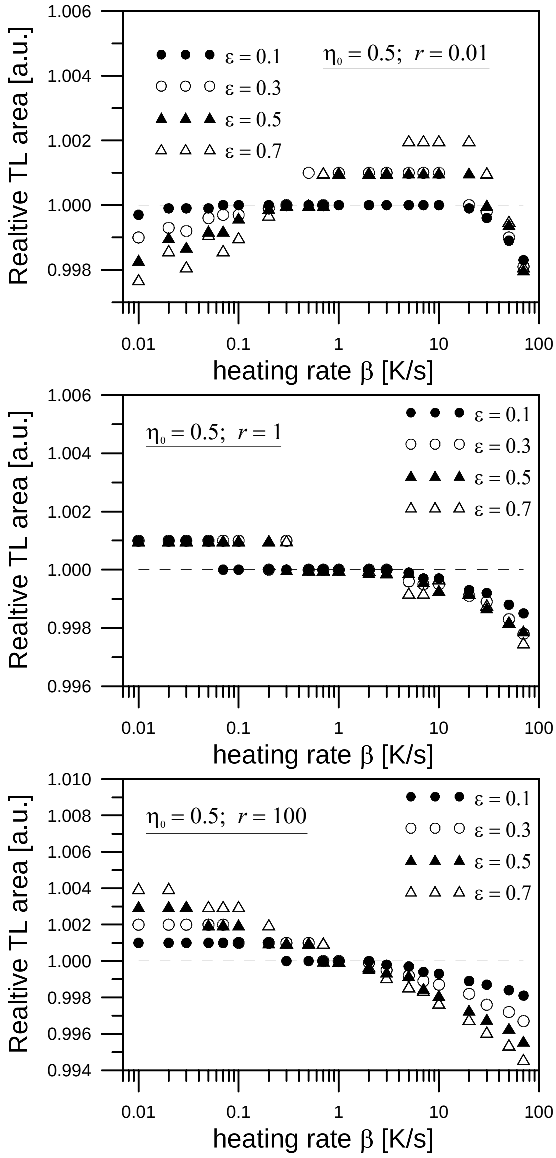

Fig. 4. Relative area under TL curve calculated for different heating rates β and various ε according to the eq. (3). Results for initial filling of traps $\eta_0 = 0,5$ and various retrapping coefficients. Other parameters the same as for fig. 2

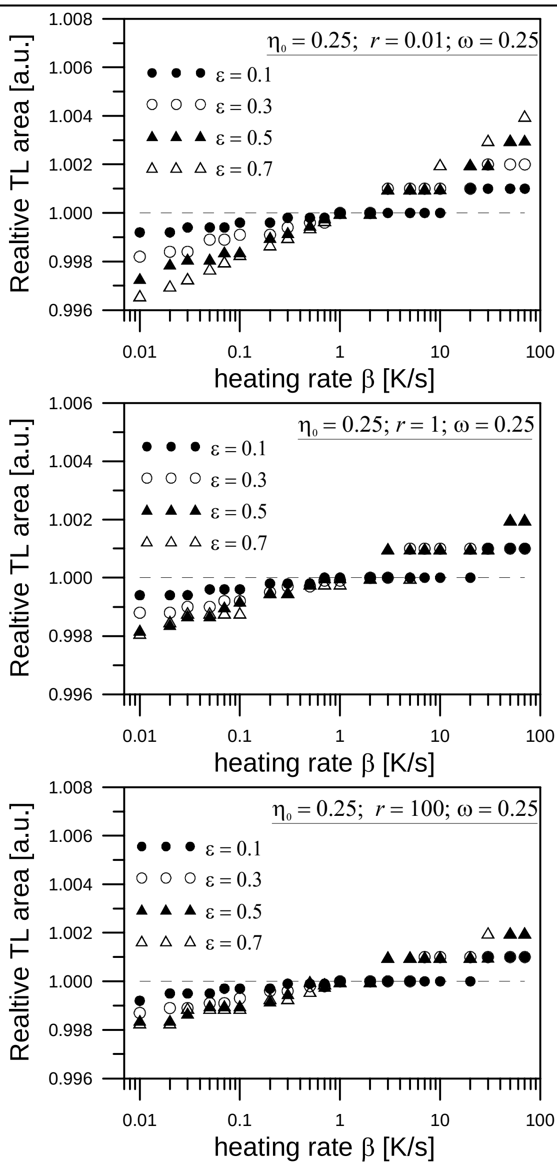

Fig. 5. Relative area under TL curve calculated for different heating rates β and various ε according to the eq. (3). Results for initial filling of traps $\eta_0 = 0,25$, in the presence of thermally disconnected traps $\omega = M/N$ and for various retrapping coefficients. Other parameters the same as for fig. 2

In this figure it seems that the area is always constant irrespective of the heating rate applied. However, more detailed analysis shows some discrepancies. It means that the assumed invariance is only approximate. To show the discrepancies we plotted the relative TL area, relating it to the average area over all heating rates for a given ε. The heating rate β was ranged from 0,01 to 70 K/s. Other parameters used for calculations are the following: trap activation energy $E = 1\,\mathrm{eV}$, recombination coefficient $B = 10^{12}\ \mathrm{cm^3 s^{-1}}$, trap density $N = 2\cdot 10^{15}\ \mathrm{cm^{-3}}$ and the frequency factor $\nu = 10^{10}\ \mathrm{s^{-1}}$. Figures 3–5 were calculated for various values of the retrapping coefficient $r \equiv A/B$. Fig. 3 presents data for full initial filling of traps $\eta_0 = 1$ and no thermally disconnected traps $M = 0$. Fig. 4 presents data for partial filling of traps $\eta_0 = 0,5$, also without thermally disconnected traps $M = 0$. The last set of diagrams (fig. 5) presents data for partial initial filling $\eta_0 = 0,25$ with the same concentration of thermally disconnected traps $\omega \equiv M/N = 0,25$.

For all presented diagrams, the discrepancy is very small - less than 1%, but typically much better. Therefore, we may state, that the integral (3) is approximately invariant with respect to the heating rate, with a high accuracy. This observation gives us an additional tool for investigating TL kinetics.

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1. *Chen R., McKeever S.W.S.* Theory of Thermoluminescence and Related Phenomena. Singapore, 1997. World Scientific.

КІЛЬКІСНА ОЦІНКА ПІКІВ ТЕРМОЛЮМІНЕСЦЕНЦІЇ

Й. Оржеховський[1], А. Мандовський[2]

[1]*Вища фахова школа Станіслава Стачіца*
вул. Шкільна 12, 27-200 Старачовіце, Республіка Польща
[2]*Інститут фізики, Університет Яна Длугоша*
вул. Армії Крайової 13/15, 42200 Ченстохова, Республіка Польща

Описано явище термолюмінесценції в межах комплексних кінетичних моделей. Показано залежності форми термолюмінесцентних кривих від величини нагрівання.

Ключові слова: термолюмінесценція, діелектрики, пастки, рекомбінація.

КОЛИЧЕСТВЕННАЯ ОЦЕНКА ПИКОВ ТЕРМОЛЮМИНЕСЦЕНЦИИ

И. Оржеховский[1], А. Мандовский[2]

[1]*Вищая профессиональная школа Станислава Стачица*
ул. Школьная 12, 27-200 Старачевице, Республика Польша
[2]*Институт физики, Университет Яна Длугоша*
ул. Армии Краевой 13/15, 42200 Ченстохова, Республика Польша

Описано явление термолюминесценции в пределах комплексных кинетических моделей. Показаны зависимости формы термолюминесцентных кривых от величины нагревания.

Ключевые слова: термолюминесценция, диэлектрика, ловушки, рекомбинация.

Стаття надійшла до редколегії 04.06.2008
Прийнята до друку 25.03.2009