PRACE NAUKOWE Wyższej Szkoły Pedagogicznej w Częstochowie
Seria: FIZYKA, CHEMIA 1992 z. IV

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THEORY AND NUMERICAL SIMULATION OF THERMALLY STIMULATED CURRENTS DUE TO DISCHARGE OF EXCESS CHARGE CARRIERS

Classical equations describing thermally stimulated currents (TSC) [1, 2, 3], because of their mathematical complexity, have no analytical solutions in general case. For the sake of simplicity, usually made assumption is to neglect retrapping processes during thermal release of trapped carriers. Then, assuming also constant life-time of charge carriers in the conduction band, one obtains formula first derived by Randall and Wilkins [4]

$$I(T)=\sum_{i=1}^{p} I_{oi} \exp\left[-\frac{E_i}{kT}-\frac{\nu_i}{\beta}\int_{To}^{T}\exp\left(\frac{-E_i}{kT'}\right)dT'\right] \tag{1}$$

where p is the number of trapping levels, k the Boltzmann constant, β the heating rate, T is the sample temperature, E_i and ν_i stand for the trap depth, and the frequency factor, respectively, I_{oi} stand for constants. In this case TSC spectrum is simply a sum of several peaks due to individual trapping levels. However retrapping, when occurs, generates nonlinear perturbation. There have been efforts to take approximately into account this effect [5, 6], but the problem is still far from beeing satisfactorily solved. The aim this work is to present model calculations, which in a different way take into account retrapping effects. Let us consider TSC experiment on the following conditions:

1) there is only one type of charge carriers in the sample
2) the whole observed current originates from space-charge carriers trapped in the sample.

Considering only „first-order approximation" which allows us to neglect detailed transport equations, we can write set of equations describing carrier kinetics in the form:

$$\begin{cases} \dfrac{dn_i}{dt} = -n_i \nu_i \exp\left(\dfrac{-E_i}{kT}\right) + n_c(N_i - n_i) v S_i & (2a) \\ n_1 + n_2 + \ldots + n_p + n_c + n_z = \text{const.} & (2b) \\ I = I(n_c) & (2c) \end{cases}$$

Here v denotes the thermall velocity of carriers, N_i and n_i denote the concentrations of trap levels and trapped cariers, respectively, n_c denotes the concentration of carriers in the conduction band, n_z stands for the number of the carriers which have left the sample, and S_i stands for the capture cross-section of the i-th trap level. Equations (2a) and (2b) describe simply kinetics of trapping processes and charge conservation law, respectively. Equation (2c) expresses the fact, that there is known a dependence of the observed current I on actual number of carriers in the conduction band. We assume, that this relation can be rewritten in inverted from, i.e. $n_c = n_c$ (I). From (2a) results

$$n_i(t) = N_i \exp\left[-\int_0^t \left(\nu_i \exp\left(\frac{-E_i}{kT}\right) + n_c v S_i\right) dt'\right] \times$$

$$\times \left\{\eta_{oi} + \int_0^t n_c v S_i \exp\left[\int_0^{t'} \left(\nu_i \exp\left(\frac{-E_i}{kT}\right) + n_c v S_i\right) dt''\right] dt'\right\}, \quad (3)$$

where η_{oi} stands for the relative initial filling of the i-th trap level. After differentiating of (2b), and substituting (2a), we have

$$\frac{dn_z}{dt} = -\sum_{i=1}^{p} \frac{dn_i}{dt} - \frac{dn_c}{dt} =$$

$$= -\sum_{i=1}^{p} \left[n_i\left(\nu_i \exp\left(\frac{-E_i}{kT}\right) + n_c v S_i\right) - N_i n_c v S_i\right] - \frac{dn_c}{dt} \cdot \quad (4)$$

This result can be combined with (3) to give

$$I = \sum_{i=1}^{p} \left\{qN_i \exp\left[-\int_0^t \left(\nu_i \exp\left(\frac{-E_i}{kT}\right) + n_c v S_i\right) dt'\right] \times\right.$$

$$\times \left\{\eta_{oi} + \int_0^t n_c v S_i \exp\left[\int_0^{t'} \left(\nu_i \exp\left(\frac{-E_i}{kT}\right) + n_c v S_i\right) dt''\right] dt'\right] \times \quad (5)$$

$$\left.\times \left[\nu_i \exp\left(\frac{-E_i}{kT}\right) + n_c v S_i\right] - qN_i n_c v S_i\right\} - q\frac{dn_c}{dt}$$

where $I = qdn_z/dt$ is the TSC current. For insulators and most of semiconductors holds $qdn_c/dt \ll I$. Then, omitting this term, and taking into account relation $T = T_o + \beta t$, one finnally comes to the equation

$$I(T)=\sum_{i=1}^{b}\left\{qN_i\exp\left[-\frac{1}{\beta}\int_{To}^{T}\left(\nu_i\exp\left(\frac{-E_i}{kT'}\right)+n_c\{I\}vS_i\right)dT'\right]\times\right. \tag{6}$$

$$\times\left[\eta_{oi}+\frac{1}{\beta}\int_{To}^{T}n_c\{I\}vS_i\exp\left[\frac{1}{\beta}\int_{To}^{T'}\left(\nu_i\exp\left(\frac{-E_i}{kT''}\right)+n_c\{I\}vS_i\right)dt''\right]dt'\right]\times$$

$$\left.\times\left[\nu_i\exp\left(\frac{-E_i}{kT}\right)+n_c\{I\}vS_i\right]-qN_in_c\{I\}vS_i\right\}.$$

Here $n_c=n_c\{I(T)\}$ is assumed to be known. This formula can be applied first of all to the curve fitting procedure, but let us try to solve another problem: how can we obtain the shape of the curve from equation (6), when all parameters are known?. The answer on this question is very important because the fundamental set of differential equations (2a) is of stiff type, so most conventional numerical methods for solving them become inappropriate. Using integral equation (6) as the starting point, the problem of simulation appears to be easier. For solving them we can propose the following iteration procedure

$$\bar{I}_{m+1}(T)=\psi\{I_m(T)\}. \tag{7}$$

Here ψ denotes the right-haud side of equation (6). If one puts $I_o(T)\equiv 0$, then $I_1(T)$ agrees with Randall and Wilkins formula (1), that is to say describes 'no retrapping' case. To check usefulness of the formula (6), there have been done numerical calculations with the usually made assumtion $n_cvS_i=\alpha\nu_iI(T)$, where α stands for a constant. For the calculation of integrals appearing in (6) the usual trapezium algorithm was used. The computer program was written in Turbo Pascal 3.0. The calculations were performed on IBM PC/XT compatibile computer with the aid of an 8087 math coprocessor. There is no analytical nor numerical evidence for the convergence of (7) in every case but in most cases of physical importance, this iteration procedure has turned out to be numerically convergent. Examples are shown on figs 1 and 2. It is clearly seen on fig. 2, that the iteration stabilizes very quickly for the initial part of a curve, but for stabilization of the high – temperature region of the diagram much more iterations is required.

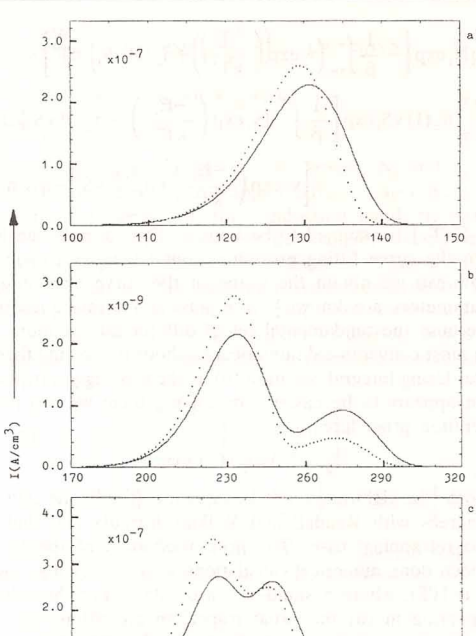
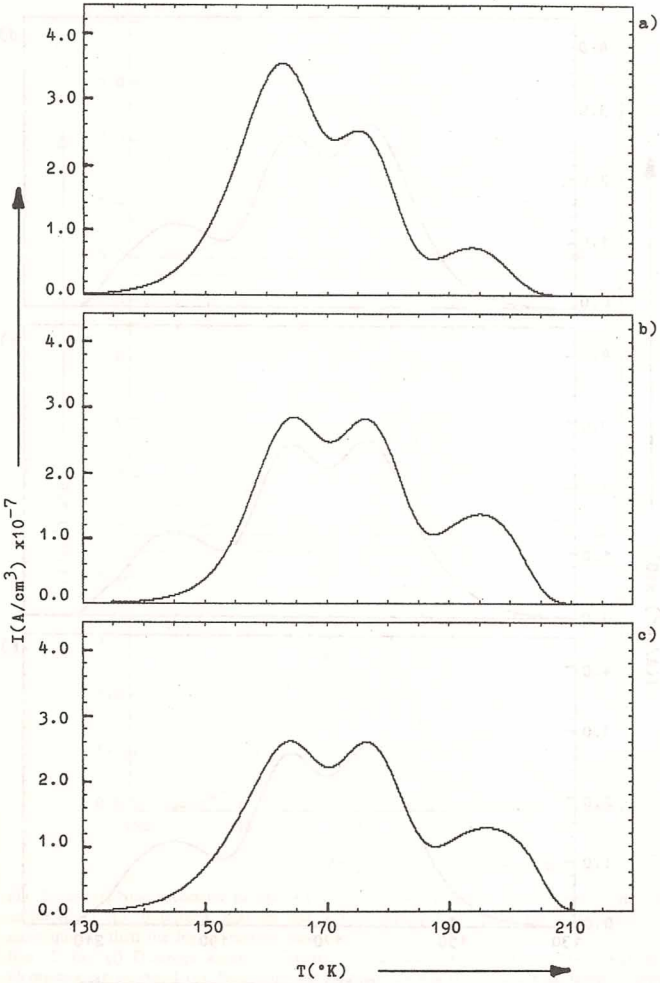
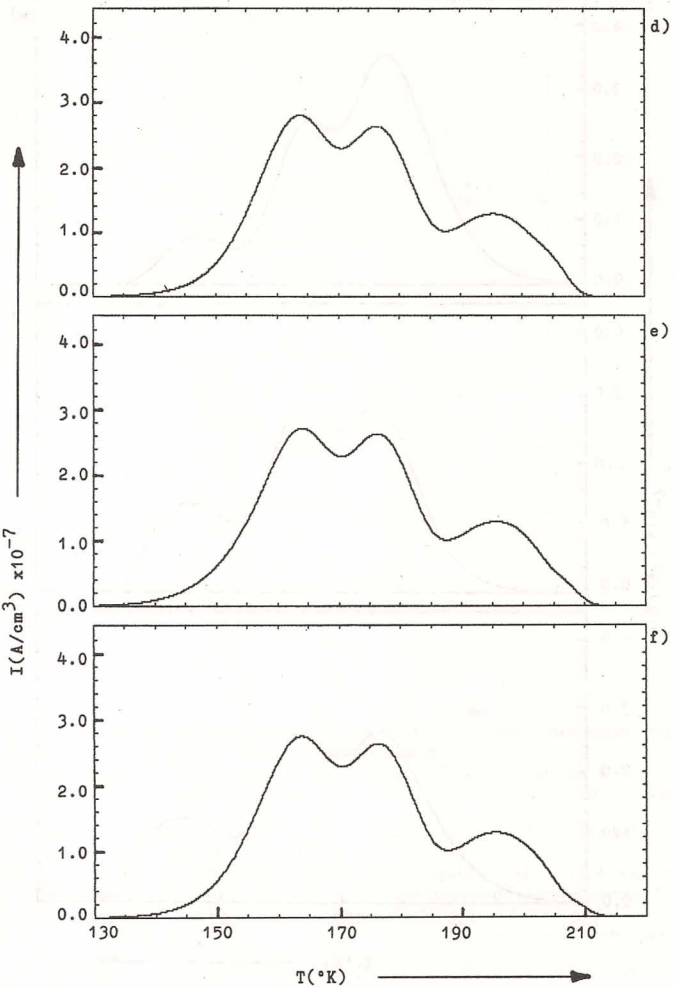


Fig. 1. TSC curves for one, two and three trapping levels, (...) calculated from Randall and Wilkins formula; (—) calculated numerically using algorithm (7):
a) $E=0.3\,eV$, $N=5\cdot10^{14}\,cm^{-3}$, $\nu=5\cdot10^{9}\,s^{-1}$, $\eta_o=0.8$, $\beta=0.05\,K/s$, $\alpha=2\cdot10^{-6}\,cm^3\,A^{-1}$
b) $E=(0.4,\ 0.47)\,eV$, $N=(10^{13},\ 10^{13})\,cm^{-3}$, $\nu=(2\cdot10^{6},\ 2\cdot10^{6})\,s^{-1}$, $\eta_o=(1,0.2)$, $\beta=0.05\,K/s$, $\alpha=0.1\,cm^3\,A^{-1}$
c) $E=(0.37,\ 0.41,\ 0.5)\,eV$, $N=(7\cdot10^{14},\ 10^{15},\ 3\cdot10^{14})\,cm^{-3}$, $\nu=(3\cdot10^{9},\ 5\cdot10^{9},\ 8\cdot10^{10})\,s^{-1}$, $\eta_o=(0.8,\ 0.5,\ 0.5)$, $\beta=0.05\,K/s$, $\alpha=3\cdot10^{-7\,cm3}\,A^{-1}$

Rys. 1. Krzywe TSC dla jednego, dwu i trzech poziomów pułapkowych, (...) obliczone ze wzoru Randalla i Wilkinsa, oraz (—) wyliczone numerycznie przy wykorzystaniu algorytmu (7):
a) $E=0.3\,eV$, $N=5\cdot10^{14}\,cm^{-3}$, $\nu=5\cdot10^{9}\,s^{-1}$, $\eta_o=0.8$, $\beta=0.05\,K/s$, $\alpha=2\cdot10^{-6}\,cm^3\,A^{-1}$
b) $E=(0.4,\ 0.47)\,eV$, $N=(10^{13},\ 10^{13})\,cm^{-3}$, $\nu=(2\cdot10^{6},\ 2\cdot10^{6})\,s^{-1}$, $\eta_o=(1,0.2)$, $\beta=0.05\,K/s$, $\alpha=0.1\,cm^3\,A^{-1}$
c) $E=(0.37,\ 0.41,\ 0.5)\,eV$, $N=(7\cdot10^{14},\ 10^{15},\ 3\cdot10^{14})\,cm^{-3}$, $\nu=(3\cdot10^{9},\ 5\cdot10^{9},\ 8\cdot10^{10})\,s^{-1}$, $\eta_o=(0.8,\ 0.5,\ 0.5)$, $\beta=0.05\,K/s$, $\alpha=3\cdot10^{-7}\,cm^3\,A^{-1}$


a)
b)
c)
4.0
3.0
2.0
1.0
0.0
I(A/cm^3) x10^{-7}
130
150
170
190
210
T(°K)


d)
e)
f)
4.0
3.0
2.0
1.0
0.0
I(A/cm^3) x10^{-7}
130
150
170
190
210
T(°K)

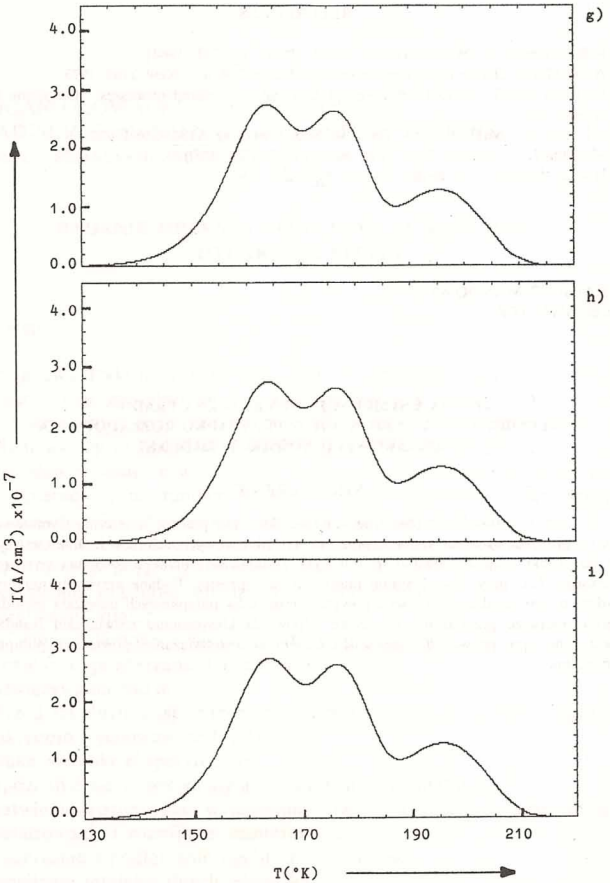


Fig. 2. (a)÷(i) Nine successive iterations (7), $I_o(T)\equiv 0$ was assumed. Parameters are the same as for fig. 1 (c). It is seen, that the low – temperature part of the curve stabilizes much more quickly then the high – temperature one.

Rys. 2. (a)÷(i) Dziewięć kolejnych iteracji (7) dla których przyjęto $I_o(T)\equiv 0$. Parametry identyczne jak na rys. 1 (c). Widoczna jest znacznie szybsza stabilizacja niskotemperaturowej części widma.

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TEORIA I SYMULACJA NUMERYCZNA PRĄDÓW TERMICZNIE WYMUSZONYCH W PRZYPADKU ROZŁADOWANIA NADMIAROWYCH NOŚNIKÓW ŁADUNKU

STRESZCZENIE

W pracy wyprowadzono równanie opisujące kinetykę prądów termicznie stymulowanych (TSC) w przypadku rozładowania (depolaryzacji) nadmiarowych nośników ładunku wstrzykniętych do próbki. Zaproponowano sposób wykorzystania otrzymanego równania do symulacji procesorów TSC przy wykorzystaniu metody iteracji prostej. Podane przykłady numeryczne świadczą o tym, że dla większości typowych parametrów pułapkowych powyższa metoda jest zbieżna. Pierwsze przybliżenie iteracyjne odpowiada klasycznemu rozwiązaniu Randalla – Wilkinsa, następne pozwalają uwzględnić efekty nieliniowe związane z powtórnym pułapkowaniem nośników.