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AN EXTENSION OF THEORETICAL DESCRIPTION OF SPACE-CHARGE-LIMITED CURRENTS IN INSULATORS*

J. Godlewski and J. Kalinowski

Institute of Physics, Technical University of Gdańsk, 80-952 Gdańsk, Poland

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The usual description of steady-state space-charge-limited currents in insulators with a continuous trap level distribution assumes the quasi-Fermi level E_F to be a sharp demarcation line at any temperature, with charge carrier traps below being filled and those above being empty. In addition this level is limited to $E_F \gg kT$. This paper describes a new approach, which avoids these assumptions and is more suitable for general discussions and approximate solutions. Conditions leading to analytical solutions are briefly discussed in terms of an exponential trap distribution.

1. INTRODUCTION

THE THEORY of steady-state space-charge-limited currents (SCLC) for insulators with a continuous trap level distribution has been developed for the cases characterized by neglecting trapped carriers above the quasi-Fermi level E_F, as it would be at 0 K (see, e.g. [1, 2].

The additional assumption $E_F(x) \gg kT$ has limited applications of the theory to the conditions with relatively low concentration of free carriers. Although general features of the current–voltage characteristics interpreted according to this theory are correctly described under these assumptions, in some cases only qualitative agreement can be expected. These are for ultra-high purity materials. Space-charge-limited currents are becoming of increasing interest in ultra-high purity single crystals, since the main source of traps are structural inhomogeneities. For such samples one may envisage low content of shallow traps and consequently, high concentration of free carriers.

In the light of these possibilities, it is desirable to embark upon a detailed description of SCLC including the occupancy of traps above the quasi-Fermi level at any position in the energy gap of an insulator.

In the present paper we restate and extend some of previously reported relationships between the principal parameters such as free- and trapped-charge carrier densities or/and mainly the current–voltage characteristics.

2. MATHEMATICAL FORMULATION

The following calculations are based on the assumptions that the capture cross-section (s) for free carriers is independent on trapping level depth, and that the rate of thermal release for all trap energies E is given by

$$P(E) = \nu \exp(-E/kT), \tag{1}$$

where ν is the collision factor considered to be independent of E.

If the density of charge trapping states per unit energy range is denoted by $h(E)$ then under equilibrium conditions

$$P(E)\,\mathrm{d}n_t(E) - n_f vs\,[h(E)\,\mathrm{d}E - \mathrm{d}n_t(E)] = 0, \tag{2}$$

where n_f is the concentration and v the thermal velocity of free carriers, $n_t(E)$ denotes the concentration of trapped carriers.

A general form of $n_t = n_t(n_f)$ relation can be obtained by use of equation (2), expression (1) and integration [3],

$$n_t = n_f vs \int_0^\infty \frac{h(E)}{\nu \exp(-E/kT) + n_f vs}\,\mathrm{d}E. \tag{3}$$

Equation (3) is considered to yield n_t for a given n_f and from it n_t can be calculated for an arbitrary distribution of charge traps.

In studies of low-mobility insulators, particularly organic molecular crystals, two types of continuous trap distributions are used: the exponential distribution of traps proposed by Rose [4] and the Gaussian distribution proposed by Croitoru and Grigorescu [5]. However, most of the experimental results reported in the literature cannot be unambigously interpreted within either of the two models; for this reason, in the further calculations we will use the exponential distribution leading to a relatively convenient analytical expression for the current (j) – voltage (V) dependences.

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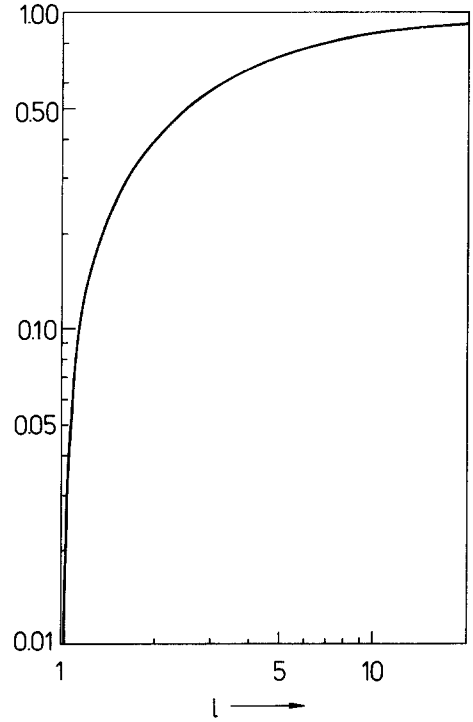

Fig. 1. Calculated l-dependence of the ratio (11).

According to Rose [4]

$$h(E) = \frac{H}{kT_c} \exp(-E/kT_c). \tag{4}$$

H is the total trap concentration, and T_c is the characteristic temperature of the distribution greater than the measuring temperature T.

Inserting (4) into (3) and substituting $\nu/v s = N_{\text{eff}}$ equal to the effective density of states in the band considered, and $l = T_c/T > 1$ one obtains (see Appendix)

$$n_t \cong \frac{H}{l}\left(\frac{n_f}{N_{\text{eff}}}\right)^{1/l} \times \left\{\pi \operatorname{cosec}(\pi/l) - [(N_{eff}/n_f)^{1-1/l}(1-1/l)]^{-1}\right\}. \tag{5}$$

This form of the relation $n_t = n_t(n_f)$ is valid if free carriers occupy only a small fraction of the states in the band ($n_f/N_{\text{eff}} \ll 1$), i.e. Boltzmann approximation for the free carriers.

We seek a solution for the equations

$$\frac{\mathrm{d}F(x)}{\mathrm{d}x} = \frac{e}{\epsilon\epsilon_0} n_t(x) \tag{6}$$

and

$$j = n_f(x) e\mu F(x) \tag{7}$$

with

$$V = \int_0^d F(x)\,\mathrm{d}x \tag{8}$$

and the boundary condition $F(0) = 0$.

Here $F(x)$ is the electric field strength; ϵ, ϵ_0 are the sample and vacuum permitivities, respectively; μ is the charge carrier mobility; e the elementary charge, d is the thickness of the sample, and V is the applied voltage.

We have neglected the free charge contribution to the total charge density and the diffusive contribution to the total current (see Appendix C in [1]).

From equations (5) to (8) we obtain

$$j = \frac{N_{\text{eff}} e\mu}{H^l}\left(\frac{\epsilon\epsilon_0}{e}\right)^l \left[\frac{l^2 \sin(\pi/l)}{(l+1)\pi}\right]^l \left(\frac{2l+1}{l+1}\right)^{l+1} \frac{V^{l+1}}{d^{2l+1}}. \tag{9}$$

We note that according to the above mentioned assumption $n_f/N_{\text{eff}} \ll 1$ and with $l \gtrsim 1.05$

$$\pi \operatorname{cosec}(\pi/l) \gg [(N_{\text{eff}}/n_f)^{1-1/l}(1-1/l)]^{-1} \tag{10}$$

so that the second term in the curly brackets of (5) could be neglected.

3. DISCUSSION

In the case of a solid with an exponential distribution of traps, it has been shown that a change in SCLC results from the continuous distribution of trapped carriers around the demarcation energy of E_F. This change as compared to the current density given by Mark and Helfrich [1]

$$j_{\text{M-H}} = \frac{N_{\text{eff}} e\mu}{H^l}\left(\frac{\epsilon\epsilon_0}{e}\frac{l}{l+1}\right)^l \left(\frac{2l+1}{l+1}\right)^{l+1} \frac{V^{l+1}}{d^{2l+1}},$$

can be expressed by the ratio

$$\frac{j}{j_{\text{M-H}}} = \left[l\frac{\sin(\pi/l)}{\pi}\right]^l = \alpha \tag{11}$$

which depends on temperature T and the characteristic trap parameter T_c ($l = T_c/T$) (see Fig. 1). For the typical range of l at room temperature ($1.5 \lesssim l \lesssim 20$; e.g. [5]) the ratio (11) changes from $\alpha \approx 0.25$ to $\alpha \cong 1$. This means that the current density in a sample with a rapidly varying distribution function $h(E)$ is overestimated by a factor of 4 when calculated according to $j_{\text{M-H}}$.

However, for ultra-high purity samples, especially at higher temperatures, one can expect l as low as, for example, 1.05. This gives $\alpha \cong 0.04$ and means that $j_{\text{M-H}} \cong 25j$. This factor over one order of magnitude is of importance in applications of the current–voltage characteristics to study charge carrier traps and, in particular, to verify the "compensation rule" [6–8].

4. APPENDIX

In deriving expression (5) the following substitution into (3) has been used

$$\frac{N_{\mathrm{eff}}}{n_f} \exp(-E/kT) = x, \tag{A1}$$

and in this way we obtain

$$n_t = \frac{H}{l}\left(\frac{n_f}{N_{\mathrm{eff}}}\right)^{1/l} \int_0^{N_{\mathrm{eff}}/n_f} \frac{x^{1/l-1}}{x+1}\,\mathrm{d}x. \tag{A2}$$

To proceed further it is convenient to use the equality

$$\int_0^{N_{\mathrm{eff}}/n_f} f(x)\mathrm{d}x = \int_0^{\infty} f(x)\mathrm{d}x - \int_{N_{\mathrm{eff}}/n_f}^{\infty} f(x)\mathrm{d}x. \tag{A3}$$

Then, for $N_{\mathrm{eff}}/n_f \gg 1$, the second integral in the right-hand side of (A3) becomes an elementary one. The first integral in this side of (A3) can be expressed by beta-function (B) as it is given in [9].

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