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SPACE-CHARGE-LIMITED CURRENTS AS AN INDICATOR OF NON-UNIFORM CHARGE TRAPS DISTRIBUTION IN THIN FILM DIELECTRICS: NUMERICAL SOLUTIONS

Space charge limited currents in inhomogeneous thin film insulating systems are studied by means of numerical methods. Calculations for two spatial distribution of traps are presented. The results confirm that the influence of charge traps at the emitter is much stronger than those at the collector. The case of illumination of the emitter is also analyzed. It turns out that it is possible to find the valued of parameter describing the exponential decay of trap distribution at the emitter and the surface trap concentration for the case of illuminated sample. The paper summarizes the data concerning possibility of determination of trap distribution at the emitter in thin film insulators using photo-enhanced space-charge-limited current measurements.

Keywords: space charge limited currents, thin films, charge traps.

1. INTRODUCTION

Thin film insulators and semiconductors are basic elements of numerous microelectronic devices. For instance the surface trapped charge influences strongly C-V characteristics of MOS capacitors [1]. Presence of surface trapped charge plays a significant role in both metal-semiconductor and metal-insulator junctions [1, 2] influencing not only their capacity but also their I-V characteristics as well. On the other hand a non-uniform spatial charge trap distribution can be also found in inhomogeneous polymeric media with continuously changing refractive index which may present unique and useful optical properties [3]. Such polymeric materials are called graded index polymers. Many practical applications of such inhomogeneous polymeric

materials has been reported [4, 5]. Such graded index polymers are often obtained by diffusion of guest molecules into host polymer network. Guest (or impurity) molecules in a host molecular solids form local localised states (traps) both for charge carriers and excitons [6, 7, 8, 9, 10]. The depth of electron traps due to impurity molecules is given by [6]:

$$E_t^e = (A_G)_{guest} - (A_G)_{host} \tag{1}$$

where A_G is the electron affinity. If $E_t^e > 0$ the electron trap is formed, for $E_t^e < 0$ we have to do with the electron antitrap. The depth of local states for holes is given by the difference of ionization energies of the guest and host molecules respectively. It has been shown that the spatial profile of impurities in some graded index polymers obtained by diffusion of guest molecules is not in agreement with Fick's equation, for instance for acrylonitryle diffusing into polystyrene [11]. The above examples show how important is an independent and reliable experimental possibility to find the spatial distribution of charge traps in thin film materials. It has been shown by means of computer analysis that space charge limited currents (SCLC) and photo-enhanced SCL currents can be used to determine the spatial distribution of charge traps in some thin film systems. This paper is to summarize the results with special reference to thin organic films.

2. INFLUENCE OF NON-UNIFORM DISTRIBUTION OF CHARGE TRAPS ON SCL CURRENTS IN THIN FILM INSULATOR

2.1. Basic assumptions of calculations

Space charge limited currents in insulators with uniform spatial distribution of charge traps is a subject of numerous papers [12-17], but very few papers refer to SCL currents in thin film insulators with non-uniform trap distribution [18-22]. The conclusions resulting from the available analytical solutions may be summarized as follows:

1. Non-uniform spatial distribution of deep traps influences both the current-voltage and the current-thickness characteristics [18, 19].
2. Traps at the emitter strongly influences the current characteristics of a thin film system, the influence of traps at the collector is usually negligible [18].
3. The non-uniform spatial distribution of shallow traps should not influence the shape of the current-voltage curves distinctly and the current-thickness dependence is of the form [19]:

$$j \propto \frac{1}{L_{eff}^{3}} \tag{2}$$

where L_{eff} is the effective sample thickness defined as follows:

$$L_{eff} = \left\{ \frac{3}{2} \int_0^L \left[\int_0^z g(x)dx \right]^{\frac{1}{2}} dz \right\}^{\frac{2}{3}} \tag{3}$$

where L is the sample thickness, g(x) is the function of the spatial distribution of traps.

The problem of SCL currents in a thin film insulator is defined by the Poisson equation:

$$\frac{dF(x)}{dx} = \frac{e}{\varepsilon\varepsilon_0}\left(n_f(x) + n_t(x)\right) \tag{4}$$

and the continuity equation:

$$j = en_f(x)\mu F(x) \tag{5}$$

where F(x) is the electric field, e is the electron charge, ε and ε_0 are relative permittivity and the permittivity of free space, j is the current density, $n_f(x)$ and $n_t(x)$ are the concentration of free and trapped charge carriers, μ is the mobility of charge carriers. For the purpose of the numerical procedure Eq. (5) was differentiated with regard to x (assuming j(x)=const), so we get:

$$\frac{dn_f}{dx} = -\frac{n_f}{F}\frac{dF}{dx} \tag{6}$$

The solutions for two spatial distributions of traps were obtained and analyzed:

$$N_t(x) = N_1 e^{-\frac{x}{D}} + N_0 \tag{7}$$

for exponential decay of trap concentration at the emitter, and

$$N_t(x) = N_1 e^{-\frac{L-x}{D}} + N_0 \tag{8}$$

for the exponential decay of traps at the collector to confirm the difference between the influence of traps placed at the two electrodes. N_0 is the uniform concentration of traps typical of the material investigated, N_1 is the trap concentration at the very surface, D is the decay parameter. Finally, the SCL currents for the distribution given by eq. (7) for illuminated emitter will be

presented to show how to find the parameter of the exponential distribution D. The occupation of traps for the dark currents is given by:

$$n_t(x) = \frac{N_t(x) + N_o}{1 + \frac{N_e}{gn_f}\exp(\frac{-E_t - E_c}{kT})} \tag{9}$$

and for the photo-enhanced SCL currents is of the form [23]:

$$n_t(x) = \frac{N_t(x) + N_o}{1 + \frac{N_e}{gn_f}\{\exp(\frac{-E_t - E_c}{kT}) + \frac{A\kappa I(x)}{\nu}\}} \tag{10}$$

N_e is the effective density of states in the conduction band, g is the degeneracy factor. E_t is the energy of the trapping level and E_c is the energy of the bottom of the conduction band, A is the quantity connecting the light intensity I(x) with free carriers generation ($A = 10^{-22}$ m^{-3} was assumed for the presented calculations, how to estimate A see [12]), κ is the absorption coefficient, ν is the thermal collision factor. The light intensity as a function of penetration distance is given by:

$$I(x) = I_0 \exp(-\kappa x) \tag{11}$$

I_0 is the incident light intensity.

The numerical procedure was tested for the trap-free case, for which the analytical solution of the SCL currents is known (eq.(12)). Both the current-voltage and the current-thickness characteristics obtained from the numerical

$$j = \frac{9}{8}\mu\varepsilon\varepsilon_0\frac{V^2}{L^3} \tag{12}$$

solutions proved to be in agreement with theoretical predictions. The thickness of all films investigated was taken to be equal to 6 μm.

2.2. Influence of traps at the emitter and at the collector

Fig. 1 shows the current-voltage characteristics of a film for the spatial trap distribution given by eq. (7). Easily detected change of slope of the current-voltage curve occurs at the voltage close to 5 V. The intensity of the change depends on the value of N_1, the concentration of traps at the very surface. For the value $N_1 = 2\cdot10^{20}$ m^{-3} the deviation from the slope 2 characteristic of the trap-free case becomes easily detectable. In the case of trap-free insulator the thickness dependence of the current density is given by:

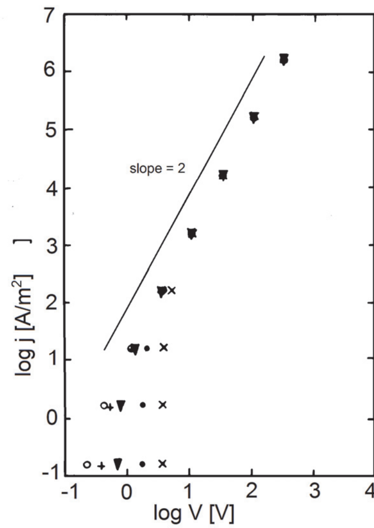

Fig. 1. Current-voltage characteristics of a film with trapped charge distribution $n_t(x) = N_1\exp(-x/D)$. D = 0.1 µm. Sample thickness L = 6 µm. n_1: o $5\cdot10^{19}$ m^{-3}, + 10^{20} m^{-3}, ▼ $2\cdot10^{20}$ m^{-3}, ● $5\cdot10^{20}$ m^{-3}, x 10^{21} m^{-3}. For the higher voltages the slope of the calculated I-V characteristics is equal to 2 resulting from the SCLC equation for trap-free case.

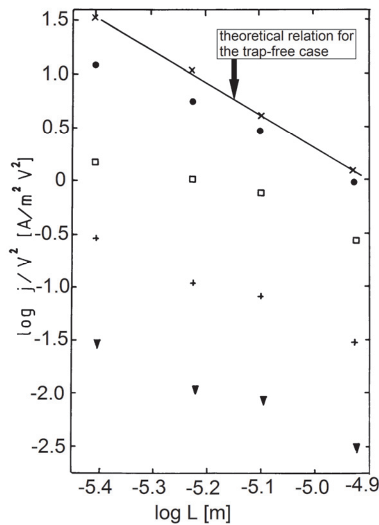

Fig. 2. Thickness dependence of current density in a film with trap distribution $n_t(x) = N_1\exp(-x/D)$. D = 0.1 µm. Sample thickness L = 6 µm. D = 0.1 µm. $N_1 = 10^{21}m^{-3}$. j: ▼ 0.16 Am^{-2}; + 1.6 Am^{-2}; □ 16 Am^{-2}; ● 160 Am^{-2}; x 1600 Am^{-2}. The full line shows the theoretical prediction given by eq.(13).

$$\log\left(\frac{j}{V^2}\right) = -3\log(L) + \log\left(\frac{9}{8}\mu\varepsilon\varepsilon_0\right) \tag{13}$$

Fig. 2 shows the thickness dependence of the current density obtained for the trap distribution given by eq.(7). The full line depicts the theoretical thickness dependence for the trap-free case resulting from eq.(13). According to the theoretical predictions resulting from analytical solutions the influence of the traps at the collector should be much weaker than those at the collector. Results presented in Fig. 3 confirms that. Only very weak influence of the traps for the highest concentration $N_1 = 10^{21}$ m^{-3} leads to detectable change of slope of the I-V curve at the lower voltages.

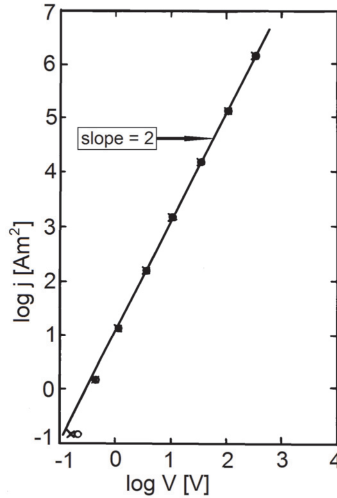

Fig. 3. Current-voltage characteristics of a film with trapped charge distribution $n_t(x) = n_1\exp(-(L-x)x/D)$. D = 0.1 μm. Sample thickness L = 6 μm. n_1: o 10^{21} m^{-3}, x $5\cdot10^{20}$ m^{-3}. All smaller values of the n_1 give points exactly on the full line. The slope of the full line is 2.

It results from the above data that the traps at the emitter influence not only the shape of current-voltage characteristics but the thickness dependence of SCL current as well. For both exponential and Gaussian energetic trap distribution and uniform spatial trap distribution the current-voltage characteristics should be given by [24]:

$$j \propto \frac{V^{l+1}}{L^{2l+1}} \tag{14}$$

where l is a parameter depending on the energetic distribution of traps and the temperature. Both the equation (14) and the thickness dependence of current in small-grain polycrystalline p-quaterphenyl films are not in agreement with

theoretical predictions [25] which may suggest that the SCL currents are influenced by non-uniform trap distribution in these films. However, SCL currents detected in so-called oriented p-quaterphenyl films [26] show typical results characteristic of trap-free case. The oriented films are of comparatively good crustal structure, so no deep traps neither in the volume nor at the emitter may be expected to exist.

2.3. Determination of the spatial trap distribution at the emitter

Fig. 4 shows the I-V characteristics for a number of various surface trap concentrations characteristic of typical partially disordered organic molecular

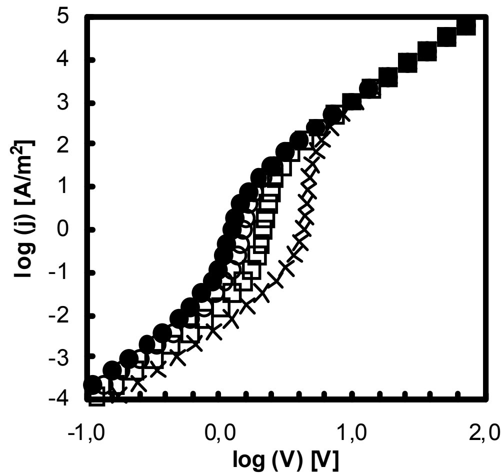

Fig. 4. SCL current-voltage relations for various surface concentrations of traps.
• $N_l = 0$; o $N_l = 10^{20}$ m^{-3}; □ $N_l = 3\cdot10^{20}$ m^{-3}; x $N_l = 10^{21}$ m^{-3}; $N_o = 10^{19}$ m^{-3}. $E_t = 0.65$ eV.

crystals [27, 28]. The trap depth $E_t = 0.65$ eV is also typical of polycrystalline structures of simple aromatic hydrocarbons [28]. It results from the figure that non-uniform trap distribution influences the I-V characteristics significantly. If weassume that the decay coefficient D is much smaller than the sample thickness, then there exists an unambiguous relation between the number of trapped charge carriers (per unit surface area) and the voltage for a given current density. This relation for the current density 10^{-3}Am^{-2} is shown in Fig. 5 for various incident light intensities and trap concentration decay coefficients. The relation remains unique for the surface concentration of trapped charge greater than about $3*10^{10}$m^{-2}. This means that the data presented in Fig. 5 enables to determine the surface concentration of charge traps from the voltage corresponding to a given current density. On the other hand there exists a unique relation between the

surface concentration of charge traps and the decay coefficient D if the surface concentration of charge is known.

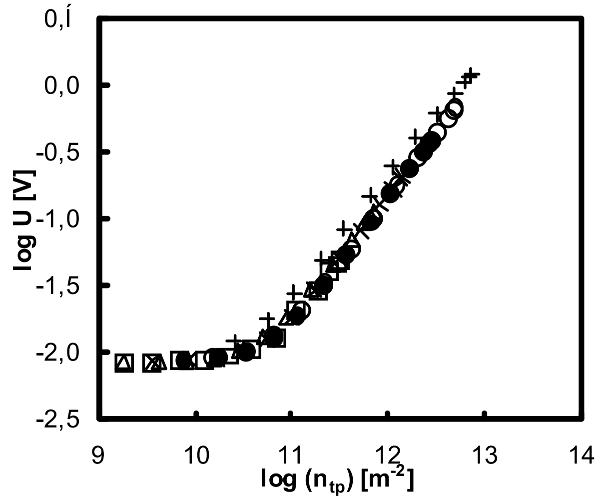

Fig. 5. The voltage (at current density 10^{-3} Am^{-2}) as a function of the number of trapped charge carriers per unit sample area for various intensities of incident light I_0 and trap concentration decay coefficients D. I_0 changes between $10^{16}\div10^{22}$ quanta/cm^{2}s. D: □ $3\cdot10^{-9}$ m; Δ 10^{-8} m; x $3\cdot10^{-8}$ m; • 10^{-7} m; o $3\cdot10^{-7}$ m; + 10^{-6} m. $E_t = 0.65$ eV. $N_1 = 10^{21}$ m^{-3}, $\kappa^{-1} = 10^{-6}$ m. T = 300 K.

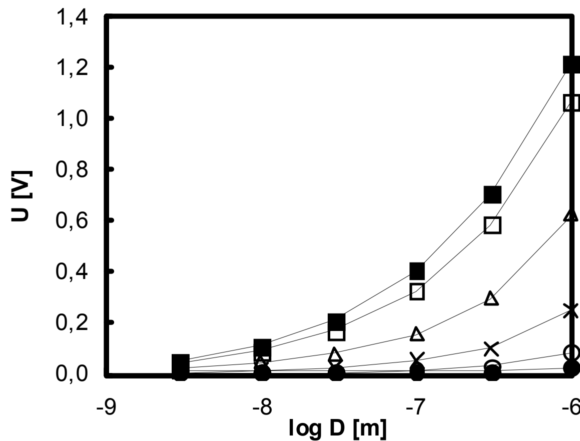

Fig. 6. The voltage U (at current density 10^{-3} Am^{-2}) as a function of the concentration decay coefficient D for various incident light intensities. I_0:□ dark current up to 10^{16} quanta/cm^2 s; □ 10^{17} quanta/cm^2 s; Δ 10^{18} quanta/cm^2 s; x 10^{19} quanta/cm^2 s; o 10^{20} quanta/cm^2 s; • 10^{21} quanta/cm^2 s. $E_t = 0.65$ eV, $N_1 = 10^{21}$ m^{-3}, $\kappa^{-1} = 10^{-6}$ m, T = 300 K.

As a result there has to exist a unique dependence between the voltage corresponding to a given current density and the decay coefficient D. Such a dependence between the voltage and the coefficient D for various light intensities is shown in Fig. 6. It results from the figure that the light intensity should not be too high, because for the high values of the light intensity the traps become unoccupied due to excitation to the conduction band.

The method of determination of the trap concentration coefficient described above works well when the surface concentration of traps is known. In case of polar impurities in non-polar host lattice this surface trap concentration should be equal to the surface concentration of polar molecules. This concentration can often be evaluated by optical reflection spectra if characteristic peaks corresponding to polar groups are detectable. The surface concentration can sometimes be estimated approximately from the solubility parameters [29]. In case of inorganic films the reciprocal of the coefficient of absorption of light κ^{-1} is usually smaller than D. In this case it is possible to determine both D nad N_1 independently from photo-enhanced SCL currents [21].

3. CONCLUSIONS

The following conclusion from the above computer analysis of the SCL currents in inhomogeneous thin film systems can be put forward:

1. Non-uniform trap distribution at the emitter influences SCL currents in solid thin film systems considerably.
2. It is possible to find the decay coefficient of the trap concentration decay at the emitter if the trap concentration at the very surface is known. However, if the absorption of light is strong enough (i.e. the reciprocal of the light absorption coefficient κ^{-1} is smaller than the decay coefficient D) then it is possible to find both the coefficient D and the surface concentration of traps N_1 independently.

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PRĄDY OGRANICZONE ŁADUNKIEM PRZESTRZENNYM JAKO WSKAŹNIK PRZESTRZENNIE NIEJEDNORODNEGO ROZKŁADU PUŁAPEK W CIENKICH WARSTWACH DIELEKTRYKÓW: ROZWIĄZANIA NUMERYCZNE

Streszczenie

Przedmiotem pracy jest numeryczna analiza prądów ograniczonych ładunkiem przestrzennym w niejednorodnych układach cienkowarstwowych. Przedstawiono wyniki obliczeń dla dwu przestrzennych rozkładów pułapek. Potwierdzono, że wpływ pułapek przy emiterze jest znacznie większy niż tych przy kolektorze. Pokazano, że stosując fotowzmocnione prądy ograniczone ładunkiem przestrzennym, można niezależnie wyznaczyć wartości stałej zaniku koncentracji pułapek i ich powierzchniowej koncentracji. Praca podsumowuje wyniki dotyczące możliwości wyznaczenia parametrów niejednorodnego rozkładu pułapek w układach cienkowarstwowych.