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NUMERICAL SIMULATION OF THE TIME-RESOLVED SURFACE PHOTOVOLTAGE AT Si-SiO_2 INTERFACES

K. Kirilov*, K. Germanova, V. Donchev, Tzv. Ivanov

Faculty of Physics, Sofia University, 5. blvd. J. Bourchier, 1164 Sofia, Bulgaria

We present a simple original algorithm for numerical simulation of super-bandgap SPV transients in semiconductors. It is applied to a p-Si/SiO_2 interface with quasi-continuously distributed non-interacting interface states. The simulated SPV time dependence is compared with experimental results, and a reasonable agreement is found.

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1. Introduction

Time-resolved super-bandgap SPV measurements can be successfully used to study the interface electronic properties and important parameters of interface states (IS) [1]. However, few detailed analysis of SPV transients have been made, because it is a complicated problem [1,2]. This refers even to the c-Si free surface and the c-Si/SiO_2 interface, which are examples of the most investigated systems. The study of this problem for these two systems is important for the following reasons: (i) The system Si-SiO_2 is a basic component of many actual device structures of microelectronics, nanoelectronics, photovoltaics etc.; (ii) The huge experience with them is used for the interpretation of results obtained from investigations of other more complicated systems.

In this work, we present a simple original algorithm which allows numerical simulations of super-bandgap SPV transients in semiconductors. It is applied to a p-Si/SiO_2 interface characterized by non-interacting IS, quasi-continuously distributed over the Si gap. The SPV time-dependence was found by numerically solving the following set of equations: (i) the continuity equations for electrons and holes; (ii) the Poisson equation; and (iii) the charge neutrality equation. The solution of these equations is carried out under two important approximations [1]: (i) The approximation of flat quasi-Fermi levels (FQL) is made; ii) The IS charge is calculated using standard Shockley-Read-Hall statistics. The simulated SPV time-dependence is compared with some experimental results, with a reasonable agreement being found.

2. Calculation details

2.1. Description of the system considered

We have considered a gateless p-Si/SiO_2 structure based on homogeneously doped and non-degenerate c-Si, at 300 K. The density of the bulk shallow acceptors is $N_A = 1.5\times10^{15}$ cm^{-3} and that of the shallow donors is $N_D = 0$. Usually, at the Si/SiO_2 interface, a depletion space charge region (SCR) occurs under thermal equilibrium. This implies that the semiconductor bands are bent downward, which corresponds to a positive surface potential, i.e. $V_{s0} > 0$ [1]. The IS reveal a quasi-

* Corresponding author: kirilowk@phys.uni-sofia.bg

continuous U-shaped distribution over the Si gap, but they do not interact in between [3]. They are assumed to be donor-like (acceptor-like) into the lower (upper) half of the Si gap [4,5].

The sample is illuminated by a short light pulse with energy 1.4 eV, corresponding to super-bandgap excitation of the Si bulk carriers. In the calculations, the contributions of the minority as well as of the majority excess carriers to the SPV formation are taken into account. This implies that each IS will interact with both bulk energy bands of Si.

2.2. The algorithm

Following the SPV definition [1], we have $\delta V_s(t)=V^*_s(t) - V_{s0}$, where V_{s0} and $V^*_s(t)$ are the surface potential barrier heights in the dark and under illumination, respectively. V_{s0} and $V^*_s(t)$ can be found from the charge neutrality equation:

$$Q_{sc}(V^*_s,t) + Q_{it}(V^*_s, t) + Q_f = 0 \qquad (1)$$

Here: $Q_{sc}(V^*_s,t)$ is the charge density in the SCR, $Q_{it}(V^*_s,t)$ is the IS charge density, and $Q_f = 1.5 \times 10^{11}$ cm^{-2} [3] is the oxide fixed charge density. Thus, for determining $V^*_s(t)$, we must know how Q_{sc} and Q_{it} depend on V^*_s and t.

2.2.1 Calculation of the charge density, Q_{sc}, in the SCR.

Assuming that the lateral dimensions of the sample are much larger than the vertical one, $Q_{sc}(V^*_s,t)$ can be found by solving the one-dimensional Poisson equation [1]. We have checked that the FQL approximation is valid in our case. Under this approximation, the Boltzmann relations which relate the SCR carrier densities to the corresponding densities in the semiconductor quasi-neutral bulk, also hold for the non-equilibrium case [1]. This makes it possible to separate the solutions of the Poisson equation and the continuity equations, thereby considerably simplifying the problem [1]. Thus, the Poisson equation for the electric potential $V(x)$ becomes:

$$\frac{d^2V(x)}{dx^2} = -\frac{e}{\varepsilon_s}\left[p_b - n_b + p_b^* \exp\left(\frac{-eV(x)}{kT}\right) - n_b^* \exp\left(\frac{eV(x)}{kT}\right)\right] \qquad (2)$$

Here, $\varepsilon_s = 11.8\varepsilon_0$ is the dielectric permittivity of Si; n_b^* , p_b^* (p_b ,n_b) are the non-equilibrium (equilibrium) free carrier densities in the bulk, i.e. at $x \geq w$ (w is the SCR width).

An explicit expression for Q_{sc} is obtained by integrating Eq. 2 from the bulk toward the surface, with boundary conditions $V(x{=}\infty) = 0$ and $dV/dx\ (x{=}\infty) = 0$:

$$Q_{sc}(V_s^*, n_b^*) = \mp \frac{\sqrt{2}\varepsilon_s kT}{eL_D^p} F^* \qquad (3)$$

$$F^* = \left[\left(\exp(-\frac{eV_s^*}{kT}) + \frac{eV_s^*}{kT} - 1\right) + \frac{n_b}{p_b}\left(\exp(\frac{eV_s^*}{kT}) - \frac{eV_s^*}{kT} - 1\right) + \frac{n_b}{p_b}\frac{\delta n(n_b^*)}{n_b}\left(\exp(-\frac{eV_s^*}{kT}) + \exp(\frac{eV_s^*}{kT}) - 2\right)\right]^{\frac{1}{2}} \qquad (4)$$

where $\delta n = \delta p$ are the excess carrier densities in the bulk.

According to Eqs. 3, and 4, Q_{sc} will depend on t via $p_b^*(t), n_b^*(t)$, and also on V_s^* .

2.2.2 Calculation of the interface state charge density Q_{it}

The dependence of the IS charge density Q_{it} on V_s^* has been derived by means of the Shockley-Read-Hall statistics and the FQL approximation [1], as follows:

$$Q_{it} = e\left[\int_{E_v}^{E_c} D_{itD}(E_{it})[1 - f_A(E_{it})]dE_{it} - \int_{E_v}^{E_c} D_{itA}(E_{it})\, f_A(E_{it})dE_{it}\right], \tag{5}$$

$$f_A(E_{it}) = \frac{v_n\sigma_{sn}(E_{it})n_b^* \exp\left(\frac{eV_s^*}{kT}\right) + v_p\sigma_{sp}(E_{it})n_1}{v_n\sigma_{sn}(E_{it})\left[n_b^* \exp\left(\frac{eV_s^*}{kT}\right) + n_1\right] + v_p\sigma_{sp}(E_{it})\left[p_b^* \exp\left(-\frac{eV_s^*}{kT}\right) + p_1\right]}, \tag{6}$$

$$n_1 = N_c \exp\left(\frac{E_{it} - E_c}{kT}\right) \quad , \quad p_1 = N_v \exp\left(\frac{E_v - E_{it}}{kT}\right) \quad , \tag{7}$$

In Eqs. 5-7: $f_A(D_{it})$ is the occupancy factor of the IS; N_c, N_v are the effective densities of states in the conduction/valence band; and v_n, v_p are the thermal velocities of electrons/holes. We obtain the donor/acceptor densities $D_{itD}(E_{it})$ and $D_{itA}(E_{it})$ as well as the electron/hole capture cross sections $\sigma_{sp}(E_{it})$ and $\sigma_{sn}(E_{it})$ of the IS by Gaussian fits to the experimental data given in [3] (Figs. 1 and 2).

According to Eqs 5 and 6, Q_{it} will depend on t via $p_b^*(t), n_b^*(t)$ and on V_s^*.

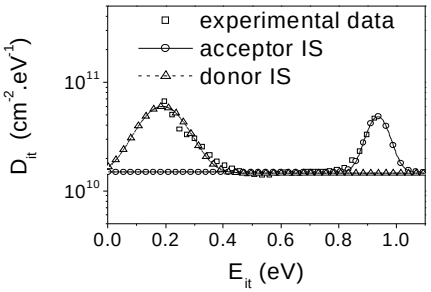

Fig. 1. IS density distribution.

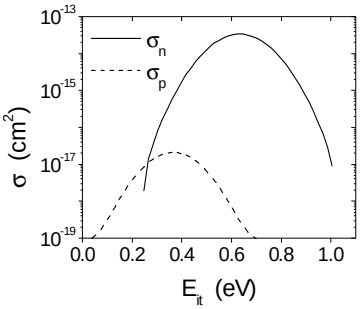

Fig. 2. IS capture cross sections.

2.2.3. Continuity equations

The time dependences of the non-equilibrium carrier densities $p_b^*(t)$ and $n_b^*(t)$ can be found by solving the continuity equations with boundary conditions: $n_b^*(0) = n_0$, $p_b^*(0) = p_0$. For simplicity, the drift and diffusion currents are not taken into account and homogeneous absorption in the whole sample is supposed. For the free carrier lifetimes, we use the values $\tau_p = \tau_n = 20$ μs [6]. The electron-hole pair generation rate per unit volume, *G(t)*, is a Gaussian with the parameters taken from [6] as follows: a total exciting energy density of 1 μJ/cm^2, a pulse duration of 0.150 μs, a time of the pulse maximum of t_0 = 0.4 μs, and absorption and reflection coefficients of 36422 m^{-1} and 0.3, respectively.

2.2.4. Calculation of the SPV time-dependence $\delta V_S(t)$

The dependencies $Q_{sc} = f[V_s^*, p_b^*(t), n_b^*(t), p_b, n_b]$ and $Q_{it} = f[V_s^*, p_b^*(t), n_b^*(t)]$ have been inserted in Eq. 1. The function $Q(V_s^*,t) = Q_{sc}(V_s^*,t) + Q_{it}(V_s^*,t) + Q_f$ is plotted in Fig. 3. Its intersection with the zero plane gives $V^*_s(t)$. From $V^*_s(t)$ and V_{s0} we find the dependence $\delta V_S(t)$.

3. Results and discussion

The exciting light pulse and the simulated SPV transient $\delta V_s(t)$ are shown in Fig. 4 by curves 1 and 2, respectively. After the beginning of the illumination, the absolute value of $|\delta V_s(t)|$ increases rapidly and reaches a maximum at the time of the light pulse maximum, $t_0 = 0.4$ μs. After that $|\delta V_s(t)|$ decreases slowly up to ~ 50 μs and then drops rapidly to zero at t = 5 ms. We could not find SPV transient measurement data for the Si/SiO_2 system in the literature. Thus, we compare our simulated $\delta V_s(t)$ curve with an experimental SPV transient (Fig. 4, curve 3), measured in [6] on a p-type c-Si free surface (100), treated in HF acid. In general, curves 2 and 3 show similar behaviour, although some discrepancies between them are seen. This result is encouraging for the difficult analysis of the time-resolved SPV, given that the numerical simulation is performed employing a simple model and the systems used in the calculations and the measurements are not exactly the same. It should be noted, however, that the IS distributions in both systems exhibit similar behaviour. Also, the simulation has been performed with parameters appropriate only to these two systems [3,5].

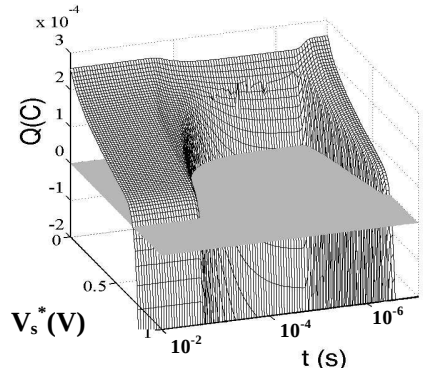

Fig. 3. The calculated function $Q(V_s^*,t) = Q_{sc}(V_s^*,t) + Q_{it}(V_s^*,t) + Q_f$ and the zero plane.

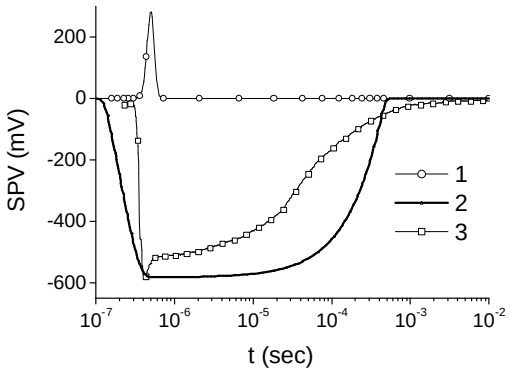

Fig. 4. 1- the exciting light pulse; 2 - the simulated and 3 - the experimental SPV transient.

4. Conclusions

The analysis carried out shows that the proposed algorithm gives a good qualitative description of the SPV kinetics in the structure considered. It could also be successfully applied to other similar structures. The time-resolved super-bandgap SPV measurements and their analysis allow the determination of important parameters of the IS. For example, the IS energy distribution could be contactlessly determined for the whole the bandgap without changing the sample from an n-type to a p-type semiconductor, or without performing SPV spectral measurements in the sub-bandgap region.

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References

[1] L. Kronik, Y. Shapira, Surf. Sci. Rep. **37**, 1 (1999) and references therein.
[2] V. Yu. Timoshenko, P. K. Kashkarov, A. B. Matveeva, E. A. Konstantinova, H. Flietner, Th. Dittrich, Thin Solid Films **276**, 216 (1996).
[3] A. G. Aberle, S. Glunz, W. Warta, J. Appl. Phys. **71**, 9 (1992).
[4] H. Flietner, Surf. Sci. **46**, 251 (1974);
[5] C. T. Wite, J. Appl. Phys. **52**, 320 (1981).
[6] V. Yu. Timoshenko, E. A. Konstantinova, Th. Ditrich, Fiz. Tehn. Poluprovod **32**, 613 (1998) (in Russian).