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Jean-Luc Maurice, Y. Marfaing

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THEORETICAL STUDY OF HIGH INJECTION EFFECTS IN EBIC MEASUREMENTS OF GRAIN BOUNDARY RECOMBINATION VELOCITY IN SILICON

J.-L. MAURICE and Y. MARFAING*

Laboratoire de Physique des Matériaux, CNRS-Bellevue, 1 Place Aristide-Briand, F-92195 Meudon Cedex, France

**Laboratoire de Physique des Solides de Bellevue, CNRS-Bellevue, 1 Place Aristide-Briand, F-92195 Meudon Cedex, France*

Abstract : The presence of carriers in the grain boundary (GB) space charge is taken into account in solving numerically Poisson's equation. This allows one, by using a schematic description of electron excitation, to investigate the theoretical behaviour of the GB recombination velocity, measured by EBIC, in high injection conditions.

1. Introduction.

The electron beam induced current (EBIC) measurement of the recombination velocity (v_s) at the grain boundaries (GB) in silicon is of interest for both fundamental research and photovoltaic industry. The link between v_s and the physical parameters of the GB traps (density N_t, energy in the gap E_t and capture cross sections for electrons and holes σ_n and σ_p) is however quite complex. We recently proposed /1/ a set of relations allowing one to deduce these parameters from EBIC measurements of v_s at varying temperature and injection level. However, for sake of simplicity, the presence of carriers in the GB space charge was either not considered (high barriers) or introduced very roughly (low barriers) and the carrier transport in this zone was also described in a schematic way.

In this paper, the presence of charge carriers in the Space Charge Region (SCR) is fully taken into account in Poisson's equation and this, in turn, allows one to use rigorous expressions for the minority and majority carrier currents (the only neglected phenomena are injection and recombination in this region). While high injection is likely to frequently occur in EBIC experiments, the present treatment has the advantage to allow, for the first time, to investigate theoretically the effects of such excitation conditions on the GB recombination velocity. This is performed on two fictional grain boundaries representative of the ones existing in p-type large grain polysilicon. The previous simplified model is simultaneously applied and comparison with the present calculation indicates its validity limits.

2. Modelling of the presence of excess carriers in the grain boundary SCR.

Poisson's equation can be written

$$\frac{d^2\varphi}{dx^2} = \frac{q^2}{\epsilon\epsilon_o}\,[p(x) - n(x) - N_A]\ , \qquad (1)$$

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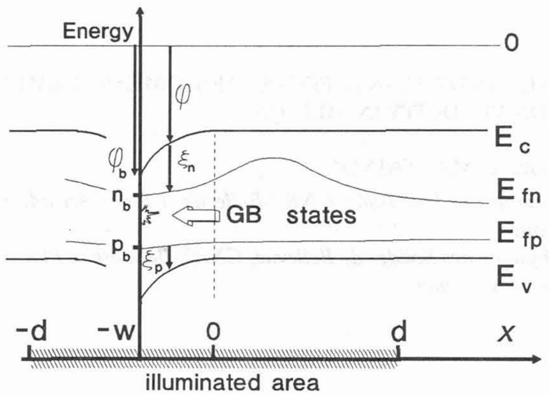

Fig.1. Energy level diagram in the vicinity of a grain boundary under local excitation. The GB is at $x = -W$; $x = 0$ corresponds to the edge of the GB space charge region. Other notations are defined in the text (the curves are arbitrary and do not reflect a real situation).

where φ is the electrostatic potential energy, x the spatial coordinate (Fig.1), q the elementary charge, $\epsilon\epsilon_o$ the silicon dielectric constant, and N_A the acceptor concentration (we assume a p-type bulk material, form and results would be symmetrically identical for n-type) . The existence of free carriers in the SCR is represented by the x-dependent concentrations of electrons $n(x)$ and holes $p(x)$,

$$n(x) = N_c \exp \xi_n/kT , \tag{2a}$$

$$p(x) = N_v \exp \xi_p/kT , \tag{2b}$$

where N_c, N_v, are the densities of states at the conduction and valence band edges respectively, kT is Boltzmann's constant times the temperature and ξ_n, ξ_p are the x-dependent chemical potentials of, respectively, electrons and holes.
Integrating equation (1) over electrostatic potential and using the Gauss theorem allows one to derive the charge of the zone (on one side of the GB) :

$$\begin{aligned} Q_{sc} &= - \frac{\epsilon\epsilon_o}{q} \left(\frac{d\varphi}{dx}\right)_{\varphi_b} \\ &= \left[2\epsilon\epsilon_o \left(N_v \int_0^{\varphi_b} \exp \frac{\xi_p}{kT}\, d\varphi - N_c \int_0^{\varphi_b} \exp \frac{\xi_n}{kT}\, d\varphi - N_A \varphi_b \right)\right]^{1/2} \end{aligned} \tag{3}$$

where φ_b is the barrier energy height ($\varphi_b = - q\, \Phi_{bi}$ of ref./1/).
The electron current in the SCR is

$$i_n = \mu_n\, n\, \frac{dE_{Fn}}{dx} , \tag{4}$$

where E_{Fn} is the electron quasi Fermi level, $E_{Fn} = \varphi + \xi_n$.
This expression can be put in the form :

$$i_n = \mu_n N_c \exp \frac{\xi_n}{kT} \left(1 + \frac{d\,\xi_n}{d\,\varphi}\right) \frac{d\,\varphi}{d\,x} . \tag{5a}$$

In steady state, this current is exactly compensated by the hole current which takes a similar form :

$$i_p = \mu_p N_v \exp \frac{\xi_p}{kT} \left(1 - \frac{d\,\xi_p}{d\,\varphi}\right) \frac{d\,\varphi}{d\,x} ; \tag{5b}$$

μ_n is the minority carrier electron mobility and μ_p is the standard hole mobility. Equation (3) has to be integrated numerically by varying φ. One then needs to know $\xi_n(\varphi)$ and $\xi_p(\varphi)$. This is obtained by extracting $d\xi_{n,p}/d\varphi$ from eqs (5a and 5b) :

$$\left(\frac{d\,\xi_n}{d\varphi}\right)_\varphi = \frac{i_n}{(\mu_n\ N_c \exp \frac{\xi_n}{kT})\ (d\varphi/dx)} - 1, \tag{6a}$$

$$\left(\frac{d\,\xi_p}{d\,\varphi}\right)_\varphi = \frac{i_n}{(\mu_p\ N_v \exp \frac{\xi_p}{kT})\ (d\varphi/dx)} + 1, \tag{6b}$$

where we have used the relation $i_n + i_p = 0$. The quantity $(\frac{d\varphi}{dx})_\varphi$ is deduced from eq.(3) taking $\varphi_b = \varphi$.

3. Current continuity and electrical neutrality.

The current given in (5a) is equal by continuity on the one hand to the recombination current (i) at the GB which is related to the physical parameters N_t, E_t, σ_n, σ_p, and on the other hand to the current (ii) coming from the grain. Using Shockley Read Hall (SRH) theory /3,4/, current (i) is :

$$i_n = \frac{N_t}{2} \gamma_p \left(p_b n_b - n_i^2\right) / [n_b + n_1 + a\ (p_b + p_1)], \tag{7}$$

where $a = \gamma_p / \gamma_n$, $\gamma_p = v_p \sigma_p$, $\gamma_n = v_n \sigma_n$, with v_n, v_p, the thermal velocities of electrons and holes respectively; p_b, n_b are the carrier concentrations at the GB and n_1 , p_1 are respectively the electron and hole concentrations that would exist if the Fermi level were at the trap energy E_t. The current from the grain (ii) is solution of the diffusion equation for $x > 0$ /1/ and makes the link with both v_s and the excitation rate g :

$$i_n = q\ v_s\ \Delta n_o = q \frac{D_n}{L_n} \left[g \frac{L^2{}_n}{D_n} \left(1 - \exp \frac{-d}{L_n}\right) - \Delta n_o \right] ; \tag{8}$$

Δn_o is the excess carrier concentration at the edge of the space charge, D_n is the minority electron diffusivity, L_n is the electron diffusion length and d is the radius of the generation sphere /2/,

$$d(\mu m) = \frac{1}{2} \times 0.0171\ [E_b(keV)]^{1.75}, \tag{9}$$

where E_b is the beam energy.

The generation rate g is taken constant inside the interval [-d, +d] - except in the SCR where it is not taken into account - and null outside. The g value can be derived from the beam current I_b and the beam voltage E_b by assuming a uniform generation within the generation sphere :

$$g = \frac{I_b}{q} \frac{E_b(keV)}{3.7 \times 10^{-3}} \left(\frac{4}{3} \pi d^3\right)^{-1}, \tag{10}$$

where 3.7 eV is the electron hole pair creation energy.

Quite generally, electrical neutrality implies that the total charge of the SCR, 2 x Q_{sc}, is equal and opposite to the charge trapped at the GB which is given by the Schokley-Real-Hall expression /3,4/ (for a donor-like recombination centre) :

$$Q_{GB} = q\ N_t\ \frac{n_1 + ap_b}{a(p_1 + p_b) + n_1 + n_b}. \tag{11}$$

4. Solving the problem.

The parameters are E_t, N_t, σ_n, σ_p, T, E_b, I_b but only the first four are actual unknowns. However to get useful curves, we fix all of them except the beam current I_b which is allowed to increase regularly over a given range. The algorithm for a given I_b value proceeds as follows :

i) a trial value is given to Δn_o, i_n is then calculated from (8).

ii) the starting values in the integration process are $\varphi = 0$, $\xi_n(n_o + \Delta n_o)$, ξ_p $(p_o + \Delta n_o)$. The initial derivatives of φ, $\xi_{n,p}$ are calculated using (3), (6). Then φ is given a small increment $(-d\varphi)$ and new values of ξ_n, ξ_p are deduced from the above equations. The process is repeated.

iii) At each step j, Q_{sc} (eq.3) is compared to the quantity Q_{GB} (obtained by putting $n_j = n_b$ and $p_j = p_b$ in eq.11). If 2 x $Q_{sc} = Q_{GB}$, the integration over φ is terminated and the computer proceeds to iv.

iv) A new value of i_n is calculated using the expression of the recombination current at the GB (eq.(7)), from which a new value of Δn_o is deduced through (8). The whole process is iterated until the first and final values of Δn_o are equal. Finally, v_s is calculated using (8).

5. Practical results and conclusions.

The two systems chosen are grain boundaries in p-type silicon ($p_o = 10^{16} cm^{-3}$, L_n = 30 μm), with the following trap characteristics and operating conditions $E_t = E_v$ + 0.45 eV, $\sigma_n = \sigma_p = 10^{-15}$ cm^2, T = 300 K, E_b = 20 keV. The trap density N_t is put

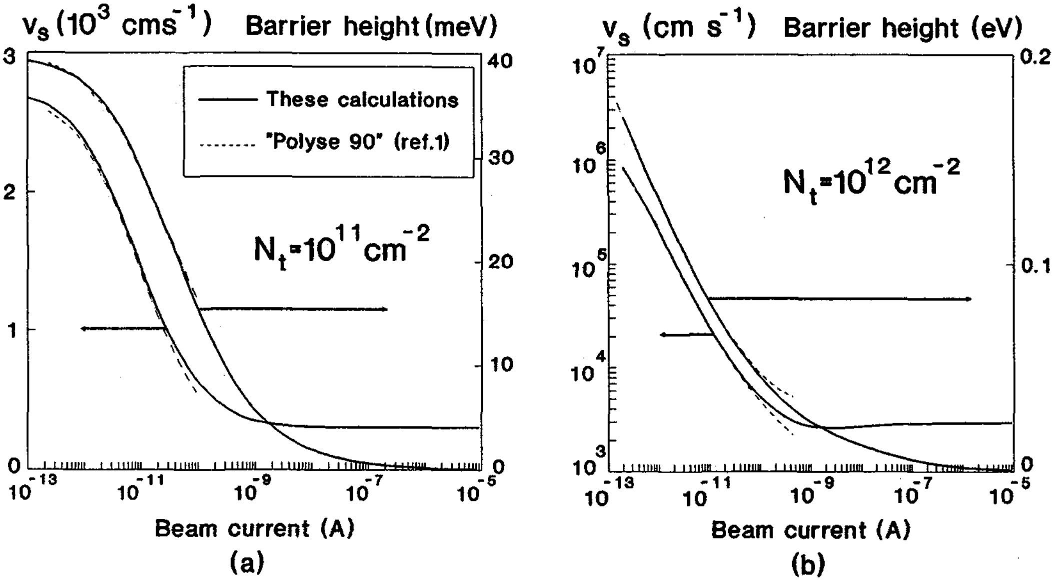

Fig.2. Recombination velocity v_s and barrier height φ_b as a function of beam current I_b at a beam energy of 20 keV, for (a) a GB with a density of hole traps near mid-gap of $N_t = 10^{11} cm^{-2}$ (φ_{bo} = 0.039 eV) and (b) a GB with $N_t = 10^{12} cm^{-2}$ (φ_{bo} = 0.28 eV), (T = 300K, kT = 0.025 eV).

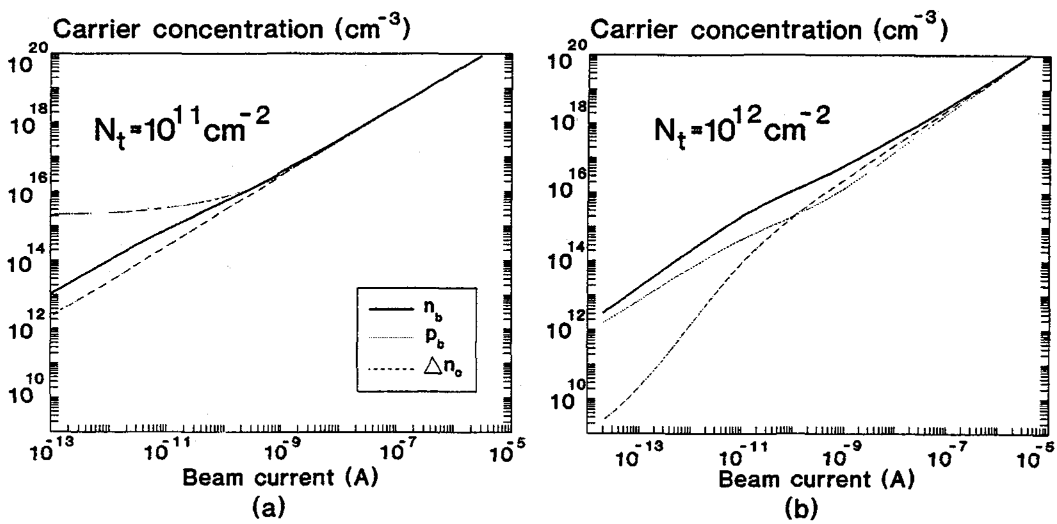

Fig.3. Concentrations of electrons (n_b) and holes (p_b) at the GB, and of excess carriers (Δn_o) at the edge of the GB space charge region, as a function of beam current I_b, for (a) the low barrier-GB (φ_{bo} = 0.039 eV) and (b) the high barrier-GB (φ_{bo} = 0.28 eV). The equilibrium concentration of holes in the grains is $p_o = 10^{16} cm^{-3}$; in case (b) the equilibrium values at the GB are $n_{bo} = 10^9$ cm^{-3} and p_{bo} = 2 x 10^{11} cm^{-3}.

equal to 10^{11} cm^{-2} (example (a)) and to $10^{12}cm^{-2}$ (example (b)) which correspond respectively to equilibrium barrier heights of 0.039 eV and 0.285 eV considering the trap states as single donors. These values have been chosen to match those generally found in the litterature /5/. The calculations have been performed over a range of beam current wider than that of standard electron microscopes by more than one order of magnitude on the low as well as on the high range sides. The behaviour of recombination velocity v_s and barrier height φ_b as a function of beam current is presented in Fig. 2. Figure 3 shows the correlated evolutions of the carrier concentrations at the GB (n_b and p_b) and at the edge of the SCR (Δn_o). Three regimes successively occur as a function of excitation rate.

* **Regime 1** corresponds to the so-called low injection regime. It is characterized by the condition $n_b << p_b$. This regime only appears in case (a) (low barrier) and for current below $\simeq 10^{-13}$A (Figs.2a and 3a). This gives a first important result : standard GBs in Si - which have barrier heights above 0.2 eV /5/ - cannot be studied in the low injection regime in usual EBIC experiments. In our example (b) (φ_{b_o} = 0.28 eV), the majority and minority carrier populations are already inversed at $I_b = 10^{-13}$A (Fig.3.b).

* **Regime 2** is an intermediate regime, which corresponds to the experimental conditions most often used ($I_b \simeq 10^{-10}$A).
The recombination velocity monotonously decreases with increasing injection. Fig.2 shows that this behaviour was already correctly described in our previous model (which indeed well fitted experimental results /1/) (dotted curves in Fig.2). The slight discrepancy at low currents in case (b) is due to the fact that the absolute limit of recombination velocity was arbitrarily put equal to the thermal velocity in /1/ ($\simeq 10^7$cm s^{-1}) while it comes out of the calculation in the present work (v_s (lim) = 2.8 x 10^6cms^{-1}). Replacing the imposed value by the calculated one corrects the discrepancy.

* **Regime 3** corresponds to the cases where the presence of carriers in the GB space charge cannot be schematically described, model /1/ does not apply anymore. This region is surprisingly characterized by a behaviour of the recombination velocity similar to that observed in the low injection case : the absence of dependence on excitation rate. This brings a second important result. The experimental observation of a constant recombination velocity over a narrow beam current range cannot be taken as a proof a low injection, one must investigate a range wide enough to include regime 2. Fig.3 indicates that electron and hole concentrations are equal in regime 3 (and equal to the excess carrier concentration), which corroborates the quasi anihilation of the barrier (Fig.2). Of course our description of the charge transport in the neutral region which considers the existence of majority and minority carriers is particularly weak in this case. However, considering ambipolar diffusion is not likely to change the behaviour observed.
Future work could be directed to a better treatment of this transport problem. However, carrying out experiments in the high injection range - which can easily be performed in any SEM - seems to be a priority.

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