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COMPUTER SIMULATION OF POLYSILICON EMITTER TRANSISTORS[1]

Péter MÁRTON

Department of Electronic Devices
Technical University of Budapest,
H-1521 Budapest, Hungary

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Abstract

In this paper, a one-dimensional model is proposed to analyse heavy doped emitters of transistors being contacted with polycrystalline silicon (polysilicon). This model is based on the Effective Recombination Velocity (ERV) approach. The effect of the polysilicon contact in Polysilicon Emitter Transistors (PETs) can be modelled as a reduced surface recombination velocity for minority carriers and the increased series emitter resistance for majority carriers. Computer simulation has been used to predict the performance of the transistor. It is pointed out that the interface between polysilicon and silicon affects the value of the current density rather than the polysilicon itself. The other physical and technological parameters, to be chosen around their reasonable values, are used as fitting parameters to simulate the real performance of the PET cited in the literature.

Keywords: Polysilicon Emitter Transistor (PET), Effective Recombination Velocity (ERV).

1. Introduction

Heavy doped polysilicon as the diffusion source of emitters or emitter contact has got wide application in advanced IC structures where its superior properties can prevail. Among them, the most significant feature is the dramatic current gain increase which can be 5–15 times larger than in conventional transistors. The reduction of the base current, which gives this beneficial property and consists mainly of the recombination current of minority carriers injected into the emitter, is mainly due to the mobility reduction of carriers in the polysilicon and the potential barrier caused by the polysilicon-silicon interface.

This phenomenon is described with calculation of the base and emitter current for a given Base-Emitter terminal voltage and technological parameters. The calculation of the base current density applies the concept

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of ERV, while in the emitter current both the tunneling and the injected diffusion currents are taken into account.

The idea of characterization of the polysilicon emitter by the ERV comes from (YU, RICCO and DUTTON, 1984), which allows to describe the effect of polysilicon emitter by a single number in respect of the base current. This value is S_E, the ERV at the interface between the monocrystalline emitter and emitter-base space-charge region (see *Fig. 2*). Physically this is a surface which can be described by its own recombination velocity. A surface having infinite recombination velocity represents the ideal drain which reduces all the excess carrier to its equilibrium level causing high recombination current. The recombination velocity of a surface is not only determined by its own value but by the space or another surface behind it, if they are at a distance of diffusion length of the carriers, and the carrier transport is possible between them. In this case, the ERV of a surface could be higher than its own value.

A simulation program has been made to evaluate the effect of the polysilicon contact using the above summarized calculation methods. Some input parameters, for example, the barrier height and thickness can be used as fitting parameters.

2. Calculation of the Base Current Density

Box Analysis of Polysilicon Grains and Grain Boundaries

It is well-known that polysilicon consists of monocrystalline grains and disordered grain boundaries. In our case the polysilicon is heavily doped, so the produced built-in electric field caused by the trapped majority carriers in the grain boundaries is negligible. By using the notations of *Fig. 1* and applying the diffusion equation to each grain and grain boundary, the current density at the ends of the grains can be determined (see Appendix A):

$$j_1 = q(a_g p_1 - b_g p_2) \,, \tag{2.1}$$

$$j_2 = q(a_g p_2 - b_g p_1) \,, \tag{2.2}$$

where p_1 and p_2 are the excess minority carrier concentrations at the edges of a grain, D_p and L_p are the hole diffusion constant and length inside the grain, being the same as in the case of monocrystalline silicon, and d_g is the grain size. a_g and b_g are constants as expressed in the Appendix A in *Eq.* (A8).

With respect to the grain boundary, *Fig. 1a* shows that it has the finite thickness (δ), and the reduction of the excess minority carrier ($p_2 > p_3$) is

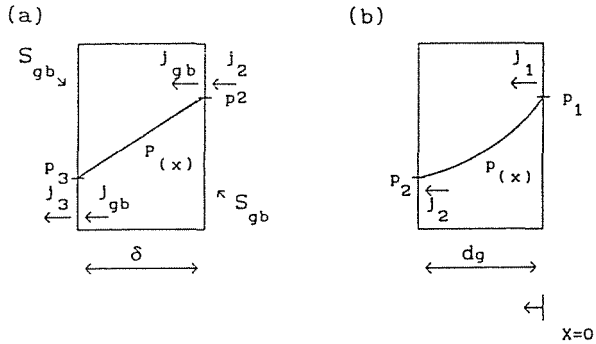

Fig. 1. Schematic diagram of the box model for the grain boundary (a), and for the grain (b)

attributed to the recombination, just like in the grains, but in this region the carrier mobility (μ_{gb}) and lifetime (τ_{gb}) have other values. The current density for the grain boundary is:

$$j_{gb} = q\frac{D_{gb}}{\delta}(p_2 - p_3) \tag{2.3.a}$$

with

$$D_{gb} = \frac{kT}{q}\mu_{gb} \,, \tag{2.3.b}$$

where δ is the width of the grain boundary. *Eq.* (2.3.a) may be rewritten as

$$j_{gb} = qT_{gb}(p_2 - p_3) \tag{2.4.a}$$

with

$$T_{gb} = \frac{kT\mu_{gb}}{q\delta} \,, \tag{2.4.b}$$

An additional recombination takes place in the surfaces between the grains and the grain boundaries, which is described by the interface recombination velocity (S_{gb}). Its definition is:

$$j_2 - j_{gb} = qS_{gb}p_2 \tag{2.5.a}$$

or

$$j_{gb} - j_3 = qS_{gb}p_3 \,. \tag{2.5.b}$$

S_{gb} is calculable from the density of states at the grain boundary, their capture cross-section and the thermal velocity of holes. (YU, RICCO and

DUTTON, 1984). Substituting (2.4.a) into (2.5) we get

$$j_2 = q(a_{gb}p_2 - b_{gb}p_3) \,, \tag{2.6}$$

$$j_3 = q(b_{gb}p_2 - a_{gb}p_3) \,, \tag{2.7}$$

where

$$a_{gb} = S_{gb} + T_{gb} \,, \tag{2.8.a}$$

$$b_{gb} = T_{gb} \,. \tag{2.8.b}$$

From one-dimensional point of view the polysilicon consists of series of boxes of grains and grain boundaries (see *Fig. 2*).

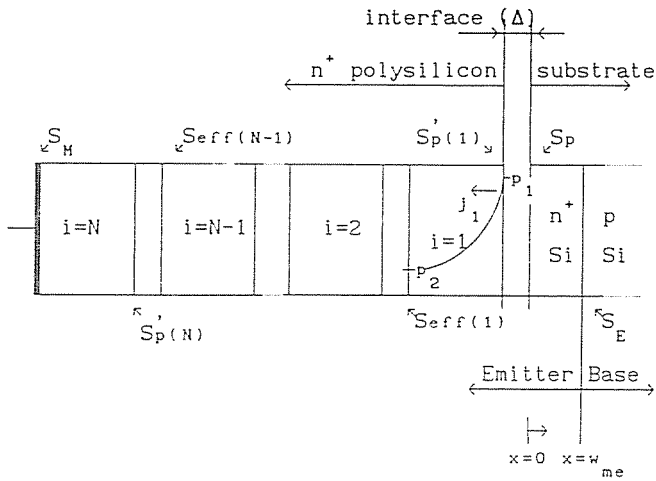

Fig. 2. One-dimensional box model of the polysilicon contact. The numbered boxes correspond to the grains, and between them there are the grain boundaries

The calculation aims at getting $S'_{p(1)}$ from S_M by stepping grain by grain from the metal contact to the polysilicon–silicon interface and counting $S'_{p(i)}$ and $S_{\mathrm{eff}(i)}$ from one another. The initial value is $S_{\mathrm{eff}(i=N)} = S_M$, the ERV of the metal surface. Index 'i' is running from N to 1. First we compute $S'_{p(i)}$ with the help of (2.9) and $S_{\mathrm{eff}(i-1)}$ with (2.10) and then 'i' is to be decreased to $N-1$ in order to evaluate $S_{p(N-1)}$ and $S_{\mathrm{eff}(N-2)}$. Generally, see Appendix A:

$$S'_{p(N)} = a_g - \frac{b_g^2}{a_g + S_{\mathrm{eff}(N)}} \,, \tag{2.9}$$

$$S_{\mathrm{eff}(i-1)} = a_{gb} - \frac{b_{gb}^2}{a_{gb} + S'_{p(i)}} \,. \tag{2.10}$$

$S'_{p(1)}$ characterizes the effect of the polysilicon layer in respect of the minority carriers in the emitter, without considering the interface between poly- and monocrystalline silicon. If $S'_{p(1)}$ is smaller than S_M, the blocking effect of the polysilicon, due to the low μ_{gb}, is dominant.

Tunneling Model of the Polysilicon–Bulk Interface

During the device manufacturing process the thin insulating layer, intentionally or not, grows between the polysilicon and the silicon. As this oxide-like layer has a wider band gap, it forms a potential barrier for both electrons and holes. This interface is in series with the emitter-base junction and the main part of the Base-Emitter voltage at intermediate bias or below falls across the p-n junction. The barrier is so high and so narrow for the carriers that they can only pass through it by tunneling. The following expression for the tunnel current is valid while the voltage drop in the interface is much smaller than $kT/q = 26$ mV, that is in intermediate bias or below (YU, RICCO and DUTTON, 1984).

$$j_p = qT_i(p_{\text{mono}} - p_{\text{poly}}) \ , \tag{2.11}$$

where T_i is the tunneling coefficient and p_{poly}, p_{mono} are the excess hole concentration at the polycrystal and the monocrystalline side of the interface, respectively.

$$T_i = q\left(\frac{kT}{2\pi m_p^*}\right)\exp(-\delta(\kappa_h m_p^*/m_0)^{1/2}) \ , \tag{2.12}$$

where m_p^* is the effective mass of holes, δ is the barrier thickness in Å, κ_h is the barrier height for holes in electron volts and m_p^*/m_0 is equal to 0.81. With (2.11) the ERV concept can be further extended to the monocrystalline side of the interface. Applying the box model to the interface, one can get the expression of the current density on the monocrystalline side of the interface with the following equation

$$j_p = qS_p p_{\text{mono}} \ , \tag{2.13}$$

where

$$S_p = S_i + \left(\frac{1}{T_i} + \frac{1}{S_i + S'_p}\right)^{-1} \ . \tag{2.14}$$

S_i denotes the original recombination velocity in the oxide-silicon interface. If its value is bigger than the second term of (1.14), the favourable effect

of the interface and the polysilicon contact cannot prevail, so the low S_i is desirable. The second term is determined by the smaller value, that is either T_i or $S'_p + S_i$. If T_i is small, which means that the oxide is thicker, the polysilicon does not play a significant role. On the other hand, if the barrier is thin enough, the polysilicon layer strongly affects the effective surface recombination velocity.

Quasi-Analytic Model of Monocrystalline Emitters

In order to be consistent with the previous box model we still use an effective recombination velocity in the emitter region defined in the following way:

$$S_{(x)} = -\frac{j_{p(x)}}{qp_{(x)}} , \tag{2.15}$$

where $p_{(x)}$ is the excess carrier concentration in the emitter. Using this definition of $S_{(x)}$, the first-order differential equation for $S_{(x)}$ can be derived (see Appendix A):

$$\frac{\mathrm{d}S}{\mathrm{d}x} = -\frac{S^2}{D_p} + \frac{1}{\tau_p} , \tag{2.16}$$

where τ_p is the hole lifetime. S at any position of x in the monocrystalline emitter can be figured out by an ordinary differential equation solver, such as Runge-Kutta method. The initial value of S is the known $S_{(x=0)} = S_p$. At $x = w_{\mathrm{me}}$, the width of the monocrystalline emitter, we get the value of $S_E = S_{(x=wme)}$. The base current, which is approximately equal to the injected minority-carrier current in the emitter, can be evaluated with the expression (2.15), where $x = w_{me}$, and $p_{(x)}$ at $x = w_{me}$ is known from the Boltzmann factor. In consequence, the expression of the base current is:

$$j_B = qS_E \frac{n_i^2}{N_{\mathrm{Deff}(wme)}} \exp\left(\frac{qV_{pn}}{kT}\right) . \tag{2.17}$$

Here, n_i and $N_{\mathrm{Deff}(wme)}$ are the intrinsic and the effective donor concentrations in the edge at the quasi-neutral emitter region near to the emitter-base junction. V_{pn} denotes the voltage falling across the $p-n$ junction.

3. Calculation of the Emitter Current Density

In our case, this calculation differs from the conventional bipolar transistors in the fact that the electron current has to flow not only across the forward biased $p-n$ junction but the oxide-like interface as well. The electrons surmount this barrier by tunneling. In order to determine this tunnel current, one has to know the voltage falling in the interface. This value is essential when the base-emitter terminal voltage is higher than 0.5–0.8 V depending on the width of the oxide layer. On the other hand, the junction voltage is also unknown. Since they are in series, the base-emitter terminal voltage is shared between the two elements, and the two currents have to be the same, that is the emitter current. To figure it out, we use a successive approximation. But it is necessary to know the two I–V characteristics of these elements.

The expression of the tunnel current density for majority carriers when a thin insulating layer is sandwiched between two heavy doped layers is as follows (YU; RICCO and DUTTON, 1984):

$$j_n = q\frac{4\pi m_n^* kT}{c_1 h^3}\exp(-b_1)\left(\frac{\pi(1-\exp(-c_1 q V_{ox})}{\sin(\pi c_1 kT)} - \exp(-c_1\xi)\ln\left(\frac{1+\exp(\xi/kT)}{1+\exp(\xi-qV_{ox})/kT}\right)\right), \tag{3.1}$$

where m_n^* is the effective mass of electrons, h and k are the Planck and Boltzmann constants, ξ is the degeneration rate, T is the absolute temperature in Kelvin, q is the elementary charge, V_{ox} denotes the voltage falling across the insulator and c_1, b_1 are constants implying the width and the height of the barrier as well as the voltage across the insulator.

The junction current is well described with the well-known expression (3.19), which is simpler if we consider the base being uniformly doped.

$$j_n = \frac{qD_n n_i^2}{W_b N_A}(\exp(V_{pn}/V_T) - 1), \tag{3.2}$$

where D_n is the diffusion constant of electrons, W_b and N_A are the width and the doping concentration of the base while V_{pn} is the voltage of the junction and $V_T = kT/q$.

The results of this method are going to be the values of V_{pn}, V_{ox} and j_n. After having these, the required V_{pn} is substitutable into (2.17). So first, the calculation of the emitter current density is needed, and afterwards comes the base current. If V_{ox} is bigger than kT/q, it indicates that the results may be false for the given Emitter-Base bias voltage.

4. Computer Simulation Results

The main difference between the normal and the polysilicon emitter transistor lies in the current gain, thus, the effect of the polysilicon contact is best described by this value. This mainly depends, among so many others, on three parameters, notably the width of the interface and the depth as well as the donor doped density of the monocrystalline emitter.

The following diagrams describe the current gain versus oxide width, while the second and the third input variable are constants or parameters as it is shown in *Fig. 3*.

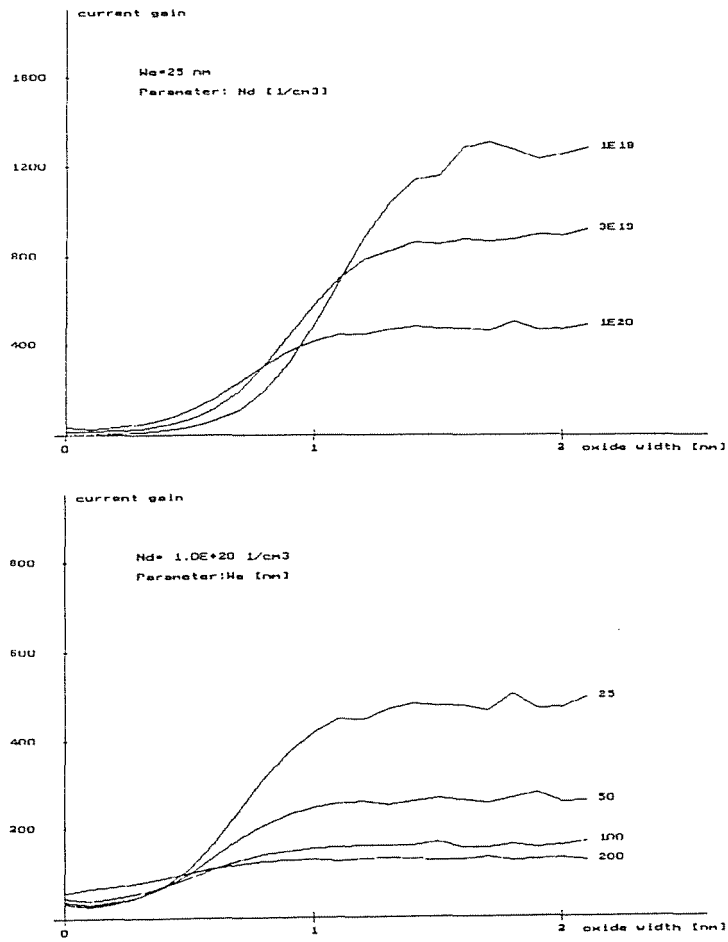

Fig. 3. Current gain versus oxide width with different emitter doped density (N_d), while the monocrystalline emitter depth (W_E) is 25 nm (a). In diagram (b) the parameter is the emitter depth, when the donor concentration is $10^{+20}1/\mathrm{cm}^3$

Fig. 3a clearly shows that increasing the oxide width from 1 to 2 nm the current gain increases dramatically, but outside of this interval the current gain begins to saturate. Its reason is that below 1 nm the tunneling probability is very close to unity, and above 2 nm the base current is only determined by $S_p = S_i$, because the second term in *Eq.* (2.14) due to the small T_i becomes much smaller than S_i. It can also be seen from this diagram that the lower the emitter donor density (N_D), the bigger the current gain increasing factor around the point of 2 nm oxide width. It is because the higher donor concentration reduces the hole lifetime and the diffusion length, which represents the same as if the monocrystalline emitter was wider causing smaller current gain. To make it clear why the wider mono-emitter layer results in lower current gain, just see *Fig. 4*. To maintain the low base current density, S_E should be as low as possible, or at least, not much higher than S_p. The more transparent the emitter, the better this requirement is fulfilled. Transparent means that the value of S_E is only slightly higher than S_p. To demonstrate the above mentioned calculation manner and its result, *Fig. 4* shows the change of ERV and the excess hole concentration through the cross-section of the transistor.

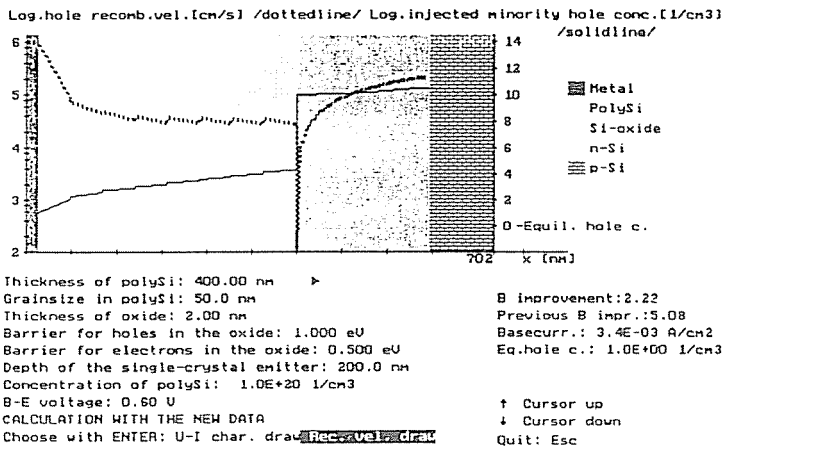

Fig. 4. ERV and concentration of minority holes from the metal contact to the E-B space-charge region. The major recombination takes place in the vicinity of oxide layer, which is also indicated by the discontinuity both in the ERV and the hole concentration curve. The same happens in the grain boundaries of the polysilicon, however, less significantly

During the calculation the base width was 0.3 μm and the base acceptor density was $5^{*}10^{+17}$ 1/cm^3. The other input parameters are shown in *Fig. 4*, and they can be altered to examine the effect of their change, and

fit the results to the published data. Strictly speaking, there are two kinds of PETs. The one which is basically a conventional bipolar transistor but the emitter contact is made of deposited poly-Si instead of Al. The so-called real PETs have quite shallow, or say 'transparent' mono-emitter, which enhances the current gain, if there is a significant oxide between the bulk and the poly-Si layer. HALEN (1983) published his experimental results for the PET manufactured with or without oxide interface. The current gain was 2000 and 100, respectively, while the emitter depth and its concentration was 20 nm and about 2^*10^{19} 1/cm^3. *Fig. 3* indicates the similar tendency if we consider that the PETs produced without interfacial oxide do have one about 0.7 nm growing inevitably during the process.

5. Conclusion

The way of describing the polysilicon emitter contact is shown to analyse DC characteristics of PETs. In this way the advantageous effect of the polysilicon is characterized by a reduced minority-carrier surface recombination velocity. This is caused by the additional scattering due to the lattice disorder in the grain boundaries and to the carrier tunneling through the polysilicon–silicon interface. The simulation result shows the differences between the transistor having about or below 1 nm oxide layer and the one having more than 2 nm oxide thickness.

Appendix

A: The diffusion equation for holes with the assumption of electric field (E) is zero, in steady state has the following form:

$$0 = \frac{\mathrm{d}p}{\mathrm{d}t} = D_p \frac{\mathrm{d}^2 p}{\mathrm{d}x^2} - \frac{p_x - p_n}{\tau_p} \ , \tag{A1}$$

where D_p is the diffusion constant of holes, τ_p is the hole lifetime, p_n is the equilibrium hole concentration in the n-doped emitter. The solution of (A1) is expected to be $p_x = p_n + \nu_x$, where the homogeneous part (ν_x) has a form of

$$\nu_x = C_1 \exp(x/L_p) + C_2 \exp(-x/L_p) \ . \tag{A2}$$

Here, $L = (D_p \tau_p)^{1/2}$, and is known as the diffusion length of holes. C_1 and C_2 are constants, which include the given conditions described in *Fig. 1b*. They are:

$$X = 0 \rightarrow p = p_1 \ , \quad X = d_g \rightarrow p = p_2 \ . \tag{A3}$$

Under these conditions we have two equations and by resolving that we gain the value of C_1 and C_2. After this step the solution of (A2) is:

$$\nu_x = \frac{p_1 \mathrm{sh}\left(\frac{d_g - x}{L_p}\right) - p_2 \mathrm{sh}\left(\frac{x}{L_p}\right)}{\mathrm{sh}\left(\frac{d_g}{L_p}\right)} . \tag{A4}$$

The relation between the hole diffusion current density and its concentration gradient is:

$$j_p = qD_p \frac{\mathrm{d}p}{\mathrm{d}x} , \tag{A5}$$

and therefore the hole current density is:

$$j = q\frac{D_p}{L_p} \frac{p_1 \mathrm{ch}\left(\frac{d_g - x}{L_p}\right) - p_2 \mathrm{ch}\left(\frac{x}{L_p}\right)}{\mathrm{sh}\left(\frac{d_g}{L_p}\right)} , \tag{A6}$$

if we take (A6) at the position of $x = 0$ and $x = d_g$, we get:

$$\begin{aligned} j_{(x=0)} &= j_1 = q(a_g p_1 - b_g p_2) , \\ j_{(x=d_g)} &= j_2 = q(b_g p_1 - a_g p_2) , \end{aligned} \tag{A7}$$

where

$$a_g = \frac{D_p}{L_p} \mathrm{coth} \frac{d_g}{L_p} ; \quad b_g = \frac{D_p}{L_p} \mathrm{csch} \frac{d_g}{L_p} . \tag{A8}$$

When it comes to transfer the recombination velocity from one interface to another one, that is from $S_{\mathrm{eff}(i)}$ to $S'_{p(i)}$, it happens in the following way (see *Fig. 1b*):

$$S'_{p(i)} = \frac{j_1}{qp_1} = a_g - b_g \frac{p_2}{p_1} , \tag{A9}$$

where we used (A7). Since the hole diffusion current is linearly proportional with the excess hole concentration at that point in the recombination velocity concept (see *Eq.* (2.15)),

$$\frac{p_2}{p_1} = \frac{j_2}{qS_{\mathrm{eff}} p_1} = \frac{b_g p_1 - a_g p_2}{S_{\mathrm{eff}} p_1} , \tag{A10}$$

from where

$$\frac{p_2}{p_1} = \frac{b_g}{a_g + S_{\mathrm{eff}}} . \tag{A11}$$

Let's put (A11) into (A9) and then $S'_{p(i)}$ is going to be deduced:

$$S'_{p(i)} = a_g - \frac{b_g^2}{a_g + S_{\mathrm{eff}(i)}} \,. \tag{A12}$$

With the similar method the same expression as (A12) can be reduced from (2.6) and (2.7) but for the grain boundaries and as the result we get (see *Fig. 1a*):

$$S_{\mathrm{eff}(i-1)} = \frac{j_2}{qp_2} = a_{gb} - b_{gb}\frac{p_3}{p_2} \,, \tag{A13}$$

where

$$\frac{p_3}{p_2} = \frac{b_{gb}}{a_{gb} + S'_{p(i)}} \,, \tag{A14}$$

finally

$$S_{\mathrm{eff}(i-1)} = a_{gb} - \frac{b_{gb}^2}{a_{gb} + S_{p(i)}} \,. \tag{A15}$$

B. From the definition of $S_{(X)}$ (2.15), and from the transport equation for holes under the condition of E (electric field) is zero follows that:

$$S_{(x)} = \frac{D_p}{p(x)}\frac{\mathrm{d}p_{(x)}}{\mathrm{d}x} \,. \tag{B1}$$

Since we need an expression for $\mathrm{d}S/\mathrm{d}x$ let's derive (B1):

$$\frac{\mathrm{d}S}{\mathrm{d}x} = D_p\frac{-1}{p_{(x)}^2}\left(\frac{\mathrm{d}p_{(x)}}{\mathrm{d}x}\right)^2 + \frac{D_p}{p_{(x)}}\frac{\mathrm{d}^2p_{(x)}}{\mathrm{d}x^2} \,. \tag{B2}$$

The first term of the right-hand side can be rewritten as $-S^2/D_p$ with the help of (B1) while the second term is related to the derivation of the hole current density expressed by the transport equation, in which the built-in electric field is due to the nonuniform emitter doping:

$$E = U_T\frac{1}{n_{(x)}}\frac{\mathrm{d}n_{(x)}}{\mathrm{d}x} = U_T\frac{\mathrm{d}\ln(n_{(x)})}{\mathrm{d}x} \,, \tag{B3}$$

so the derivation of the hole current density is:

$$\frac{\mathrm{d}j_p}{\mathrm{d}x} = qD_p\frac{\mathrm{d}^2p}{\mathrm{d}x^2} + qD_p\frac{\mathrm{d}}{\mathrm{d}x}\left(p_{(x)}\frac{\mathrm{d}\ln(n)}{\mathrm{d}x}\right) \,. \tag{B4}$$

If we perform the second term of (B4) in the right-hand side we get:

$$qD_p \frac{\mathrm{d}}{\mathrm{d}x}\left(p_{(x)} \frac{\mathrm{d}\ln(n)}{\mathrm{d}x}\right) = qD_p'\left(\frac{\mathrm{d}p_{(x)}}{\mathrm{d}x}\frac{\mathrm{d}\ln(n)}{\mathrm{d}x} + p_{(x)}\frac{\mathrm{d}^2\ln(n)}{\mathrm{d}x^2}\right), \qquad \text{(B5)}$$

where the second term of the right-hand side proves to be zero if $n_{(x)}$ is described by the exponential function of x. From the continuity equation for holes follows that (B4) is proportional to the excess hole concentration $(p_{(x)} - p_n)$ divided by the holes life time (τ_p) at steady state

$$\frac{\mathrm{d}j_p}{\mathrm{d}x} = q\frac{p_{(x)} - p_n}{\tau_p} = qD_p\frac{\mathrm{d}^2p_{(x)}}{\mathrm{d}x^2} + qD_p\frac{\mathrm{d}p_{(x)}}{\mathrm{d}x}\frac{\mathrm{d}\ln(n)}{\mathrm{d}x}. \qquad \text{(B6)}$$

Since the twofold derivation of $\ln(n)$ is not significant, with the help of (B1), (B6) has the following form:

$$D_p\frac{\mathrm{d}^2p_{(x)}}{\mathrm{d}x^2} = S_{(x)}p_{(x)}\frac{\mathrm{d}\ln(n)}{\mathrm{d}x} = \frac{p_{(x)} - p_0}{\tau_p} \approx \frac{p_{(x)}}{\tau_p}, \qquad \text{(B7)}$$

where the simplifying is under the fact that $p_{(x)} >> p_0$ in the monocrystalline emitter. From the latter (B6) equation the required value of the second term of (B2) can be expressed and substituted back into (B2). Finally, one can gain the expression of $\mathrm{d}S/\mathrm{d}x$:

$$\frac{\mathrm{d}S}{\mathrm{d}x} = -\frac{S^2}{D_p} + \frac{1}{\tau_p} - S_{(x)}\frac{\mathrm{d}\ln(n)}{\mathrm{d}x}. \qquad \text{(B8)}$$

During the numerical solution it has turned out that the last term of (B8) can be ignored due to the logarithm function of $n_{(x)}$.

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