MAPPING OF DEFECT RELATED SILICON BULK AND SURFACE PROPERTIES WITH THE ELYMAT TECHNIQUE

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The Elymat technique exploits specific properties of silicon electrolyte junctions and permits to map diffusion length as well as surface defects. New modes have been obtained by combining several measurements using Lasers with different penetration depths and/or applying a bias which is well below the value for photo current saturation. This allows to extract information about the depth dependent bulk diffusion length as well as the recombination velocities of front and back surface.

INTRODUCTION

Present and future IC technologies require low levels of lattice imperfections, especially heavy metal contamination, in the Si wafer. Fe contamination, e.g., should be below $10^{10} cm^{-3}$ in the starting material and should not go up during processing. The need for monitoring defects at this extremely low concentration level leads to the development of innovative equipment capable of generating a life time map of a wafer. Since the life time is closely related to defects in general this is often sufficient to evaluate the basic contamination level and, with some experience and luck, the contamination source [1, 2, 3, 4]. The ELYMAT (short for electrolytical metal tracer) is such a tool; in its present day configuration it is capable of delivering high-resolution maps ("Elymaps" [5]) of the bulk life time, and, as an unique feature, Elymaps of the surface recombination velocity [6].

WORKING PRINCIPLE OF THE ELYMAT AND NEW APPLICATIONS

Fig. 1 shows a schematic cross section through the "heart" of the ELYMAT, i.e. the electrolytical double cell. In essence, both sides of a wafer are in contact with an electrolyte (normally, but not necessarily, diluted HF (1% - 2%)) and, using a set of contact needles around the perimeter of the wafer, arbitrary voltages can be applied independently between the electrodes contacting the electrolytes and the front and back side of the wafer. The resulting front and back side currents are measured in the regular modes of the Elymat as a function of a local illumination with a Laser beam. The front side is defined as the illuminated side (not necessarily the polished side of a wafer). The regular modes either measure the induced photo currents at the front side (FPC-mode) or at the back side (BPC-mode). The measured currents

contain the information about the bulk diffusion length in a quantitative way as shown in detail below; cf. also [3, 6].
The unique properties of the Si-HF electrolyte junction are crucial for the existing and future applications of the ELYMAT. For a more detailed treatment the reader is referred to [6], here only the basics will be discussed using the qualitative J-U characteristics of a p-type Si HF junction as shown in Fig. 2. For n-type Si the situation is more complicated and will not be discussed; suffice it to mention that most applications are still feasible. The most important features are:
In region I of the cathodic regime of the J-U characteristics (cf. Fig. 2), the junction behaves like a very good reversely biased Schottky contact; i.e. leakage currents can be very low and break-through voltages are only determined by the resistivity of the Si. With a working point in this region, the junction collects minority carriers; this is the "saturation region" for photo currents used in the FPC or BPC mode. The very low leakage currents (easily below $5 * 10^{-6} A/cm^2$) imply that the interface recombination velocity of the Si-HF interface is very low; as is indeed the case [7]. This is essential for the quantitative evaluation of diffusion lengths.
The anodic region II (cf. Fig. 2) is only indirectly used in the regular modes. If measurements are made without the contact needles (which is advantageous and not problematic for FPC mode and in principle possible, but not yet fully understood, in the BPC mode), one side of the wafer is automatically biased anodically. The anodic regime, however, can be used for in-situ preferential etching of defects, for removing defined amounts of Si via dissolution and for some more involved techniques outlined in [8].
Of particular and recent interest is the cathodic region III. In this region the junction behaves quite different from a Schottky contact. Current flow is restricted by the associated chemical reaction (i.e. H_2 evolution). In physico-chemical language: The electrode potential is below the hydrogen overvoltage. If the voltage of the minority carrier collecting half-cell lies in region III, a certain part of the light induced minorities is unable to flow as a current into the electrolyte as they would do in the saturation region. FPC measurements in this region are called RPC mode, short for restricted photo current, and allow new insights into material properties.
In addition to juggling with the possibilities of the Si electrolyte junctions, other major parameters easily varied over several orders of magnitude are the penetration depth of the illuminated light and its intensity. The latter translates directly into the injection level of the minorities and allows "injection level spectroscopy", for details cf. [9].
Another unique feature of the ELYMAT technique is the possibility to measure the leakage currents of the junction. Whereas leakage currents are usually not welcome, and rather low for "good" Si, it has been shown in [10], that they indicate very well for processes about to run out of specification and thus are extremely useful in monitoring processes/equipment.

THEORY FOR FPC AND BPC

We consider the case where the bulk properties depend only on the depth z. In the case of homogeneous illumination of the front side of the wafer the electron concentration n_p in p-type Si is described by the second order differential equation [11]

$$D_n \frac{\partial^2 n_p}{\partial z^2} - \frac{n_p - n_{p0}}{\tau_n(z)} + \alpha F(1-R)e^{-\alpha z} = \frac{\partial n_p}{\partial t}, \tag{1}$$

with
D_n : diffusion constant,
$\tau_n(z)$: recombination time of electrons,
n_{p0} : electron concentration in thermal equilibrium,
α^{-1} : penetration depths of the Laser,
R : reflectivity of Laser beam,
F : number of incident photons per area and time.

The first term in Eq. [1] corresponds to the diffusion of the electrons. The second term describes the recombination of electrons in the bulk by a relaxation time $\tau_n(z)$, which may depend on the depth z. The third term represents the generation of electrons by the Laser beam.
For steady state condition, assuming the wafer to be uniform in mobility, doping level and lifetime, i.e. $\tau_n = \text{const}$, $D_n = \text{const}$ and $n_{p0} = \text{const}$, Eq. [1] is solved by

$$\begin{aligned} n_p(z) - n_{p0} &= a \cosh\left(\frac{z}{L}\right) + bL \sinh\left(\frac{z}{L}\right) \\ &\quad - \frac{\alpha F(1-R)\tau_n}{(\alpha L)^2 - 1}\left(e^{-\alpha z} + \alpha L \sinh\left(\frac{z}{L}\right) - \cosh\left(\frac{z}{L}\right)\right); \end{aligned} \tag{2}$$

where a and b are constants, which have to be evaluated by the boundary conditions at $z = 0$ and $z = d$ (the wafer thickness), and $L := \sqrt{D_n \tau_n}$ is the diffusion length. The current is defined by

$$J(z) = \pm q D_n \frac{\partial n_p}{\partial z}(z) \quad . \tag{3}$$

For the standard ELYMAT-modes the bias of the collecting junction is always beyond the value for current saturation. The boundary conditions for the

FPC-mode are:

$$\begin{aligned} n_p(0) - n_{p0} &= 0 \quad \text{(no electron accumulation at the front surface)} \\ \frac{\partial n_p}{\partial z}(d) &= 0 \quad \text{(no surface recombination at the back side)} \end{aligned}$$

leading to
$$\frac{J_{FPC}}{J_{max}} = \frac{1}{1-\frac{1}{(\alpha L)^2}} \frac{\cosh\left(\frac{d}{L}\right) - \frac{1}{\alpha L}\sinh\left(\frac{d}{L}\right) - e^{-\alpha d}}{\cosh\left(\frac{d}{L}\right)(1-e^{-\alpha d})} \tag{4}$$

In Eq. [4] we have neglected the surface recombination on the back side of the wafer and J_{max} is the total induced current

$$J_{max} = qF(1-R)(1-e^{-\alpha d}) \ . \tag{5}$$

For a Laser with small penetration depth ($\alpha^{-1} \approx 10\mu m$) and moderate values of $L \approx 200\mu m$, $J_{FPC} \approx J_{max}$ is nearly independent of L. The space charge region (SCR) on the front side even increases this effect because a substantial part of the electrons are induced in the SCR, where no recombination occurs. Only for $L < 50\mu m$ diffusion length measurements in the FPC mode are sensible.
The boundary conditions for the

BPC-mode are:

$$\begin{aligned}
n_p(d) - n_{p0} &= 0 \quad \text{(no electron accumulation at the back surface)} \\
D_n \frac{\partial n_p}{\partial z}(0) &= S_f n_p(0) \quad (S_f\text{: front surface recombination velocity}) \\
\text{leading to} \quad \frac{J_{BPC}}{J_{max}} &= \frac{1}{\left(1-\frac{1}{(\alpha L)^2}\right)\left(\cosh\left(\frac{d}{L}\right) + \frac{S_f L}{D_n}\sinh\left(\frac{d}{L}\right)\right)} * \\
&\left\{1 + \frac{S_f}{D_n \alpha} - \frac{e^{-\alpha d}}{1-e^{-\alpha d}}\left[\left(\frac{1}{\alpha L} + \frac{S_f L}{D_n}\right)\sinh\left(\frac{d}{L}\right)\right.\right. \\
&\left.\left. + \left(\frac{S_f}{\alpha D_n} + 1\right)\left(\cosh\left(\frac{d}{L}\right) - 1\right)\right]\right\} \qquad (6)
\end{aligned}$$

For a less penetrating Laser beam with $\alpha << d, L$ Eq. [6] reduces to

$$\begin{aligned}
\frac{J_{BPC}}{J_{max}} &\approx \frac{1 + \frac{S_f}{D_n \alpha}}{\cosh\left(\frac{d}{L}\right) + \frac{S_f L}{D_n}\sinh\left(\frac{d}{L}\right)} \qquad (7) \\
&\approx \frac{1}{\cosh\left(\frac{d}{L}\right)} \qquad \text{for } S_f \to 0 \quad , \qquad (8)
\end{aligned}$$

which shows, that the photo-current is nearly independent of the penetration depth. Especially for $S_f \to 0$ Eq. [8] gives a very simple expression for the evaluation of L. Summing up, we see that using a Laser with small penetration depth (e.g. a standard IR Laser with $\lambda \approx 820nm$ and $\alpha^{-1} = 13\mu m$) the ELYMAT technique allows a priori measurements of the diffusion length under certain assumptions:

1. The penetration depth must be small in comparison to the wafer thickness ($\alpha d >> 1$).

2. The front surface recombination S_f must be neglectable.

3. The diffusion length must be uniform in z-direction.

In consequence the diffusion length L is a simple function of J_{BPC}, J_{max} and d (Eq. [8]), which are quite easy to measure. But using only this mode for measuring L, there is no way of checking the validity of the above assumptions. The results may be misinterpreted, e.g. if $S_f > 0$ electrons recombine at the front side reducing the photo current at the back side, and thus applying Eq. [8] the bulk diffusion length seems to be reduced. Whereas the first condition can always be met and HF-passivation of the surface states usually (but not always) allows to neglect S, we loose all information about the original surface and have no way to decide, whether the bulk diffusion length is uniform or not.

COMBINATION OF IR- AND SIR-LASER MEASUREMENTS

To get additional information about the surface recombination S as well as the depth profile of the diffusion length we use an additional infrared Laser with wavelength $\lambda = 1047nm$ and penetration depth $\alpha^{-1} = 490\mu m$, which, for the sake of clear distinction from the regular $\lambda = 820\mu m$ infrared Laser, has been dubbed "strong" infrared (SIR)-Laser. This Laser induces electrons with a depth dependent concentration profile shifted towards the back side of the wafer. Therefore J_{BPC} is less sensitive to S_f and more sensitive to the diffusion length in the back half of the wafer and the photo current is a measure for an averaged diffusion length with a different weight for each Laser. If the Elymaps for IR- and SIR-Laser are similar, it is likely that the above assumptions are fulfilled.
This new Laser allows to measure diffusion lengths $50\mu m \leq L \leq 100\mu m$ with ease which were heretofore difficult to measure and thus diffusion lengths from nearly zero up to about three times the wafer thickness can now be investigated.
Most information about the diffusion length distribution of a wafer can be obtained by combining several IR- an SIR- measurements. As shown in Fig. 3 we model the diffusion length profil by a set of N points z_i with constant diffusion lenght L_i between z_i and z_{i+1}. The electron concentration $n_{p,i}$ in each region is described by Eq. [2] replacing $z \to z - z_i$ and $F \to Fe^{-\alpha z_i}$. The parameter a_i and b_i are evaluated by the surface conditions S_f and S_b and the steadiness of $n_{p,i}(z)$ and $\partial n_{p,i}/\partial z$ at the steps z_i, leading to a set of linear equation for a_i and b_i. Thus the calculated photo currents J_{BPC} and J_{FPC} are functions of the set z_i, L_i and the Laser parameters α and F.
We find the optimal parameters z_i and L_i by a least square fit, i.e. by minimizing the function

$$H(z_i, L_i, S_f, S_b) := \sum_n \left(J_{n,measured} - J_{n,calculated}(z_i, L_i, S_f, S_b)\right)^2 \tag{9}$$

where n indicates the measuring mode (FPC or BPC, in combination with α and F).
The Figs. 4a-4c show the results of such a fit for a $6\mu m$ epitaxially grown p surface layer on a p^- wafer and a model, containing one step in the diffusion length and therefore the parameters S_f, S_b, z_1, L_0 and L_1. To fit these parameters, at least 5 independent measurements of photo current are necessary, yet for the sake of reducing statistical error it seems preferable to have a greater set of measured data. We therefore measured photo currents in 6 modes: BPC IR-Laser, BPC SIR-Laser, FPC SIR-Laser and the same modes for the wafer "upside down", i.e. front and back side interchanged.
Fig. 4a shows the calculated bulk diffusion length L_1, Fig. 4b the calculated diffusion length of the surface layer L_0 (corresponding to the epitaxial layer) and Fig. 4c shows the depth z_1 of the calculated step. Obviously the bulk diffusion length is much better than the diffusion length of the surface layer. This is an unexpected result because epitaxially grown layers usually have quite good diffusion lengths, nevertheless it is in accordance with FPC measurements using a red Laser with a penetration depth of $4\mu m$.
The calculated step is about a factor 2 greater than the depth of the epi layer. This may be explained by a continous change from the low diffusion length in the surface layer to the better one in the bulk. Approximating this change by a step causes a greater stepsize than the depth of the epi layer.
The most obvious part of the bulk diffusion map is the ring, probably caused by oxigen precipitation, leading to a more complicated diffusion length profile. This ring is seen in the L_0 and z_1 map (Fig. 4b,c) as well, which may be an artifact of the fitting routine. If the diffusion length profile is much more complicated than the underlying model, even the "best" approximation may not fit very well.
Discussing this fitting problem we must bear in mind that the epi layer has only a depth of about one percent of the wafer thickness and it has a correspondingly little influence on the photo current. The calculated parameters of the surface layer are therefore not as accurate as the calculated bulk diffusion length.
The number of fit parameters of the model is restricted by the number of independent photo current measurements, indicated by FPC- or BPC-mode and different values of the penetration depth α. Increasing the number of measurements means therefore to increase the number of Lasers with different penetration depths, which is quite complicated and expensive. A much more elegant way of creating independent measurements may therefore be the change of the boundary conditions for the diffusion problem applying a bias well below the value for current saturation, which will be dicussed in the next section.

RESTRICTED PHOTO CURRENT (RPC)-MODE

In contrast to the regular modes, which measure the photo current in the saturation regime of the J-U characteristics, in the restricted photo current (RPC)-mode

the applied bias is smaller and only a part of the induced electrons, which emerge at the surface, are flowing through the semiconductor-electrolyte-junction and are measured as photo current. The current limiting process is the chemical reaction kinetics for H_2- evolution. The light generated carriers which cannot contribute to the current increase the minority carrier density in the bulk. The depth distribution of these carriers depends on the bulk diffusion length as well as on the local properties of the SCR (The situation is somewhat similar to a leaking, illuminated MOS contact).
To discuss this problem, we must know the voltage distribution across the semiconductor-electrolyte-junction: The bias $U_0 < 0$ across this junction can be split into a voltage drop U_{el} across the electrolyte in the so called Helmholtz-zone and the voltage U_s across the space charge region (SCR) of the semiconductor, or

$$U_0 = U_{el} + U_s \quad . \tag{10}$$

For the calculation of the voltage distribution we have to apply the Poisson equation obtaining a complicated differential equation, especially on the semiconductor side where we have to consider the band bending $\psi = -U_s$, caused by the voltage drop U_s, and the bending of the quasi fermi potential of the electrons Φ_n, caused by the minority current. Fig. 5 shows a qualitative plot of these model parameters.
For sake of simplicity we use the model of abrupt SCR, assuming that no recombination takes place in the SCR. The width W of the space charge region is defined by charge neutrality across the junction. For $z > W$ the electric field will be neglected; so the minority distribution is characterized by Eq. [1] discussed above.
To describe the chemically determined charge flow through the junction we apply the Buttler-Volmer equation [12], a well known equation for an electrochemical equilibrium reaction, which is approximated for $U_{el} < 0$ by

$$J(0) \approx C\, n_p(0)\, e^{-\delta\beta U_{el}} \quad , \tag{11}$$

where $0 < \delta < 1$ and $C \ll 1$ are chemically determined parameters, $\beta := q/(k_B T)$ and

$$n_p(0) = n_p(W) e^{\beta(\psi - \Phi_n)} \qquad\qquad (\psi(W) = \Phi_n(W)) \quad . \tag{12}$$

Combining the Poisson equation with Eq. [11] and [12] for a fixed value of $n_p(W)$, we get ψ, Φ_n and $J(0)$ and thus $J(W)$ by

$$J(W) = J(0) - qF(1-R)\left(1 - e^{-\alpha W}\right) \quad . \tag{13}$$

Repeating this procedure for different values of $n_p(W)$ a function

$$\tilde{S}_f(n_p(W)) := \frac{J(W)}{q n_p(W)} \tag{14}$$

can be defined, which specifies the possible boundary conditions for the minority diffusion in the bulk. Applying Eq. [14] on a given depth dependent diffusion length

distribution, there is one $n_p(W)$, which serves as a boundary condition for that distribution, and thus $n_p(W)$, $J(W)$, $J(0)$ and the depth W of the SCR are calculated. The explicit calculation will be shown in a subsequent paper, but there are some qualitative aspects, which can be presented here:
Fig. 2 shows, that we can apply a bias of about 1 V without any current flowing across the junction. In this regime the contact works almost like a perfect insulator, possibly even allowing an inversion layer at the surface. On the other hand the electrons cannot accumulate at all in a surface near layer in the saturation regime. Thus by adjusting the bias every electron concentration at the surface can be choosen in RPC-mode, which also causes a strong variation of the depth W of the SCR. Because these variations depend on the concentration $n_p(W)$ and therefore on the bulk diffusion length L, there is a strong variation of RPC photo current with the bulk diffusion length even with a red Laser ($\alpha^{-1} = 4\mu m$), which is not seen in the saturation regime (cf. Fig. 2).
Summing up, the voltage distribution across the HF-Si junction and therefore the SCR specify the boundary conditions fore the RPC-mode. In consequence, SCR determining properties like electrolyt-concentration, dotping of the wafer or surface near defects, which are not always correlated with L, may also have a strong influence on the photo current in the RPC-mode.
Fig. 4d shows a RPC-map of the above discussed wafer. Remarkable is the horizontal line through the center of the wafer and two spots: One at the right end of this line and one in the center. Neither of these structures is seen in the FPC- or BPC-measurements or in the calculated maps. Thus the reduction of photo current in these areas is not an effect of reduced diffusion length but probably induced by an inhomogeneous SCR. Variations of the photo current caused by the bulk or surface diffusion length are small in comparison.
In contrast to the above RPC-measurement Figs. 6a and 6b show an example of a wafer where the BPC- and RPC-mode deliver very similar Elymaps, which clearly indicates that bulk diffusion lengths are obtainable from RPC-Elymaps in principle.

SUMMARY AND CONCLUSION

The ELYMAT principle allows to obtain information about the internal and surface perfection of a Si wafer in several different modes. It was shown that maps of interesting properties as, e.g. surface recombination velocities or depth dependence of L, can be obtained by relating independent measurements of the well understood standard mode with the help of a complete theory,.
In addition, first results of a new mode, specific to the ELYMAT technique, were presented. This new RPC mode, although much more difficult to understand theoretically, not only offers the possibility to provide additional information about the bulk properties, but seems to have the potential to map imperfections at or very

close to the surface that are not seen in standard diffusion length maps.

ACKNOWLEDGMENTS

The authors appreciate help and encouragement from Dr. P. Eichinger

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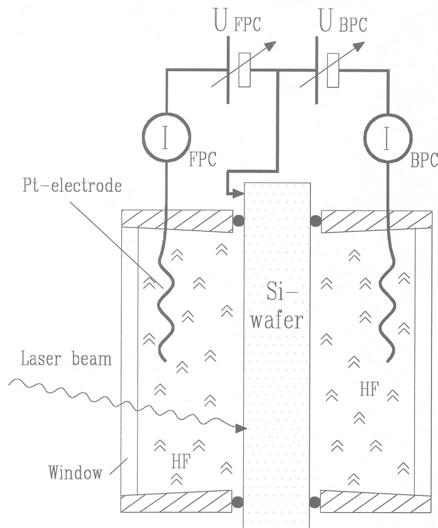

Figure 1: Schematic cross-section through the ELYMAT electrolytical double cell.

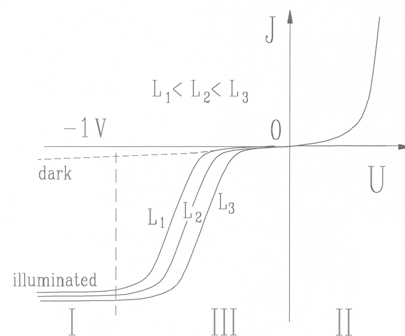

Figure 2: Typical current-voltage relationship of p-Si in contact with HF-electrolyte. The variation with L in region III is exagerated.

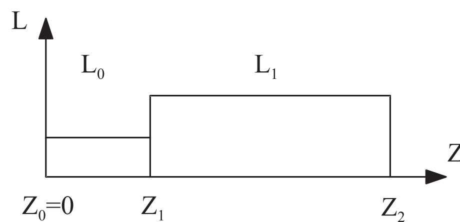

Figure 3: The model for fitting the photo current data. The depth dependence of the diffusion length profile is approximated by a set of steps.

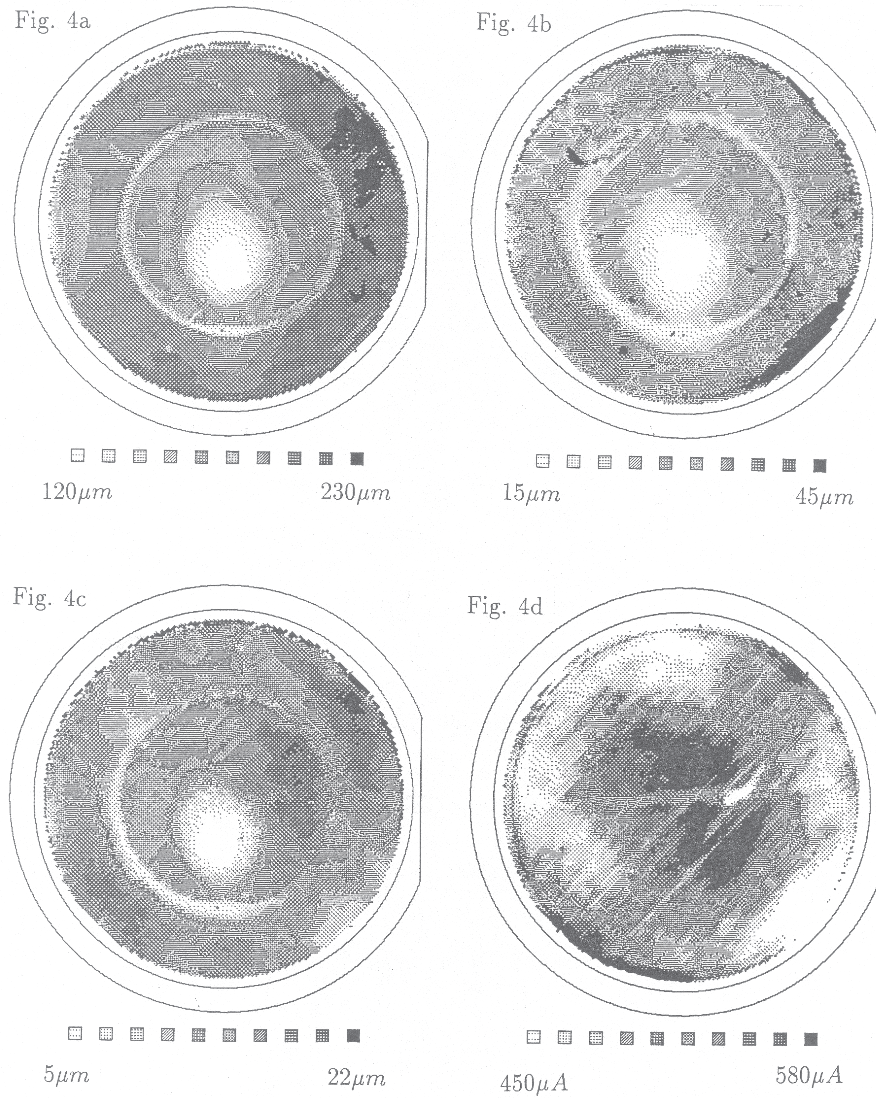

Figure 4: Elymaps of an epitaxially grown p surface layer on a p^- wafer. a) Calculated diffusion length of the bulk, b) Calculated diffusion length of the surface layer, c) Calculated depth for the step in the diffusion length profile. Figure d) shows the measured photo current in RPC-mode.

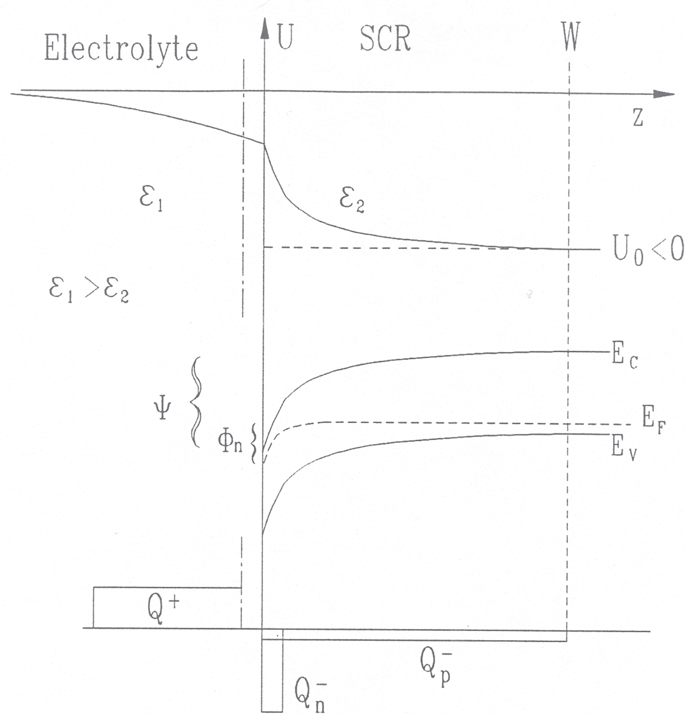

Figure 5: Qualitative voltage distribution, band bending Ψ, the quasi-Fermi potential Φ_n, and the charge distribution in the RPC mode. The depth W of the SCR is defined by charge neutralisation assuming an abrupt SCR.

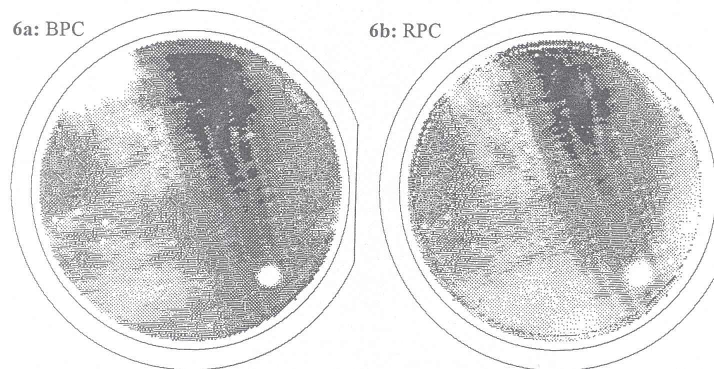

Figure 6: BPC and RPC elymaps of the same wafer showing no significant differences in the photo current. The corresponding diffusion lengths range from 200 to 600 μm.