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Differential methods for determination of deep-level parameters from recombination currents of *p*–*n* junctions

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Two techniques for determining the activation energies of centers that create deep levels in the space-charge region (SCR) of $p-n$ junctions are developed on the basis of the Shockley–Read–Hall recombination model. The proposed techniques are based on a consideration of recombination currents in the SCR for a low injection level. The first technique involves a differential analysis of the reduced recombination rate $\partial R_{np}(U)/\partial U$ and the second technique involves an analysis of the dependence $R_{np}^2(U)/\exp(qU/2kT)$. These techniques are used to analyze the current–voltage characteristics of gold-doped silicon p^+-n diodes. The gold-related deep center activation energies obtained from the current–voltage characteristics are in good agreement with the available data in the literature. © *1998 American Institute of Physics.* [S1063-7826(98)01010-2]

INTRODUCTION

Generation–recombination processes in the space-charge region (SCR) of a $p-n$ junction were first considered in Ref. 1. Using the statistics of recombination through a simple two-charge Shockley–Read–Hall center, the authors of Ref. 1 obtained a general expression for the recombination current density in the SCR (in the form of an integral over the SCR of the recombination rate). They were able to obtain analytical expressions only for some particular cases for various simplifying assumptions. The entire current–voltage characteristic (CVC) due to recombination currents in the SCR of the $p-n$ junction for a low injection level (LIL) was obtained in Refs. 2–6. Although complete agreement with the results of numerical integration of the recombination rate was not obtained, some estimates may still be considered as satisfactory.[5–7]

The approach developed in Refs. 5 and 6 allows one to determine the activation energy of deep levels, and with additional information it also allows one to determine the ratio of capture coefficients or lifetimes in the quasineutral regions. In comparison with the techniques of transient generation of carriers in the SCR of the $p-n$ junction [thermally stimulated capacitance (TSC),[8] deep-level transient spectroscopy (DLTS)[9]] which require measurements over a wide temperature interval, an analysis of the recombination current can be performed at some fixed temperature (e.g., room temperature). This leads to simpler measurements. On the basis of the method developed in Ref. 8 we developed two additional techniques of processing the recombination current in the SCR for low injection levels. What sets this work apart is the use of the computer at every stage of the process: from performing the measurements to producing the final result. The objects of study were gold-doped silicon p^+-n diodes of commercial manufacture (D-220). About these diodes (D-220) it is known that they are produced by an alloy technology, and the doping levels of the p^+ and n regions are constant (the $p-n$ junction is sharp, as is confirmed by the results of capacitance measurements. This choice was motivated by the fact that gold in silicon has been studied extensively[10] and can be used as a test of the proposed techniques.

RECOMBINATION CURRENTS IN THE SCR AND THE REDUCED RECOMBINATION RATE

Recombination currents in the SCR of a $p-n$ junction through simple two-charge deep centers are described by the expression[6]

$$i_r=\sum_{m=1}^{s}\frac{qSw(U)c_{nm}c_{pm}n_i^2\left(\exp\left(\frac{qU}{kT}\right)-1\right)N_{tm}}{2n_i\sqrt{c_{nm}c_{pm}}\exp\left(\frac{qU}{2kT}\right)+c_{nm}n_{1m}+c_{pm}p_{1m}}\times\frac{2kT}{q(U_{\text{dif}}-U)},\tag{1}$$

where $w(U)$ is the width of the SCR, s is the number of deep levels, S is the area of the $p-n$ junction, $n_{1m}=N_c\exp(-E_{mm}/kT)$, $p_{1m}=N_v\exp(-E_{tpm}/kT)$, c_n and c_p are the electron and hole capture coefficients for capture by the given center averaged over all states, N_t is the concentration of deep levels, and E_t is the position of the deep level in the band gap. $E_{tn}=E_c-E_t$, $E_{tp}=E_t-E_v$. Expression (1) holds provided the following conditions are satisfied: the deep centers are uniformly distributed over the band gap, the levels are discrete, the system is found in thermal equilibrium, illumination is absent, and tunneling transitions and recombination are controlled entirely by thermal processes.[4,5] Expression (1) was derived on the basis of the Shockley–Read–Hall theory of recombination through a simple two-charge center and differs somewhat from the expression derived in Ref. 1. This difference was discussed in detail in Refs. 4 and 7, and the derivation is given in Ref. 6; we will therefore not consider it here. The limits of applicability of expression (1) were also determined in Refs. 4–6. Each term in expression (1) is the recombination current through the corresponding (mth) deep level. Expression (1) can be represented in the form[7]

$$i_r=\frac{2kTw(U)Sn_i}{U_{\text{dif}}(u)-U}\sum_{m=1}^{s}\frac{\alpha_m\left(\exp\left(\frac{qU}{kT}\right)-1\right)}{2\zeta_m\exp\left(\frac{qU}{2kT}\right)+\zeta_m^2+1},\qquad(2)$$

where $\alpha_m=(n_{1m})/n_i)c_{nm}N_{tm}$ and $\zeta_m=(n_{1m}/n_i)\sqrt{c_{nm}/c_{pm}}$ (here we have made use of the equality $n_{1m}p_{1m}=n_i^2$). The dependences $U_{\text{dif}}(U)$ and $w(U)$ in Eqs. (1) and (2) can be found from the capacitance measurements. Thus, only the parameters α_m and ζ_m, which depend only on the nature of the deep levels, on their concentration ($c_{nm}, c_{pm}, E_{tm}, N_{tm}$), and on the material of the semiconductor (n_j), remain unknown. Earlier it was proposed to analyze the recombination currents with the help of the reduced recombination rate R_{np} (Refs. 4–6), which is defined as

$$R_{np}(U)=\frac{i_r(U)\exp\left(\frac{qU}{2kT}\right)}{Sw(U)n_i\left(\exp\left(\frac{qU}{kT}\right)-1\right)}\,\frac{U_{\text{dif}}(U)-U}{2kT}.\qquad(3)$$

From Eqs. (2) and (3) the relation between this quantity and the deep-center parameters is apparent:

$$R_{np}(U)=\sum_{m=1}^{s}R_{npm}(U)=\sum_{m=1}^{s}\frac{\alpha_m\left(\exp\left(\frac{qU}{kT}\right)-1\right)}{2\zeta_m\exp\left(\frac{qU}{2kt}\right)+\zeta_m^2+1}.\qquad(4)$$

If $s=1$ (one deep level), then Eqs. (2) and (4) are described by only two parameters, which can be found by the trial-and-error method. In general, the number of fitting parameters is $2s$. They can be found by the method of successive trial and error in each segment of $R_{npm}(U)$ for every mth deep center and successive subtraction of $R_{npm}(U)$ from the curve $R(U)$. This procedure can be done graphically[5,6] or automated. Having determined ζ_m, we easily find for fixed temperature

$$E_{tnm}=\frac{E_g}{2}-kT\ln\zeta_m+\frac{3}{4}\,kT\ln\frac{m_n^*}{m_p^*}+\frac{1}{2}\,kT\ln\frac{c_{nm}}{c_{pm}}.\qquad(5)$$

The activation energy of the mth deep level is determined to the last term, which can be found by making measurements at several temperatures. (For many centers c_n/c_p does not exceed 10^2; thus at $T=300$ K $(kT/2)\ln(c_n/c_p)\cong 0.06$ eV.) In addition,

$$\frac{\alpha_m}{\zeta_m}=\left(\frac{1}{c_{nm}N_{tm}}\right)^{1/2}\cdot\left(\frac{1}{c_{pm}N_{tm}}\right)^{1/2}=\sqrt{\tau_{n0m}\cdot\tau_{p0m}}.\qquad(6)$$

THE DIFFERENTIAL TECHNIQUE ($\partial R_{np}(U)/\partial U$)

From Eq. (4) we find $\partial R_{np}(U)/\partial U$. Differentiation gives

$$\frac{\partial R_{np}(U)}{\partial U}=\frac{q}{2kT}\sum_{m=1}^{s}\frac{\alpha_m\exp\left(\frac{qU}{2kT}\right)(\zeta_m^2+1)}{\left(2\zeta_m\exp\left(\frac{qU}{2kT}\right)+\zeta_m^2+1\right)^2}.\qquad(7)$$

It is easy to see that the function (7) has maxima. To find them we search for extrema:

$$\frac{\partial^2R_{np}(U)}{\partial U^2}=\left(\frac{q}{2kT}\right)^2\times\sum_{m=1}^{s}\frac{\alpha_m\exp\left(\frac{qU}{2kT}\right)(\zeta_m^2+1)\left(\zeta_m^2+1-2\zeta_m\exp\left(\frac{qU}{2kT}\right)\right)}{\left(2\zeta_m\exp\left(\frac{qU}{2kT}\right)+\zeta_m^2+1\right)^3}=0.\qquad(8)$$

Since we have assumed that the recombination processes proceed independently through each center, Eq. (8) is satisfied if each term in the sum is equal to zero (assumption of the technique). Thus

$$\zeta_m^2+1-2\zeta_m\exp\left(\frac{qU_{0m}}{2kT}\right)=0,\qquad(9)$$

$m=1,2,\dots,s$, where U_{0m} is the position of the maximum for the mth term. Solving the quadratic equation for ζ_m, we find

$$\zeta_m=\exp\left(\frac{qU_{0m}}{2kT}\right)+\sqrt{\left(\exp\left(\frac{qU_{0m}}{2kT}\right)\right)^2-1}\qquad(10)$$

(we have chosen the root with the ``+'' sign). If $\exp(qU_{0m}/2kT)\gg 1$, then

$$\zeta_m=2\exp\left(\frac{qU_{0m}}{2kT}\right).\qquad(11)$$

Using expression (10) or (11) for ζ_m, we find E_{tnm} using formula (5). Substituting ζ_m^2+1 from Eq. (9) in expression (7), we find that the amplitude of the mth maximum, A_m, is

$$A_m=\frac{q}{2kT}\,\frac{\alpha_m}{8\zeta_m}.\qquad(12)$$

Knowing ζ_m, it is easy to find α_m or ζ_m/α_m.

Thus, instead of finding α_m and ζ_m, it is possible by expanding R_{np} into its components to construct the dependence $\partial R_{np}(U)/\partial U$ and find ζ_m and ζ_m/α_m from the positions of the maxima (U_{om}) and the value of the function at these points. Next, using Eqs. (5) and (6), we can calculate the required parameters.

The given technique has two important advantages in comparison with the technique proposed in Ref. 5, which analyzes $\partial\gamma(U)/\partial U$ and $\gamma(U)=(2kT/q)\partial(\ln R_{np}(U))/\partial U$: first, it is necessary to construct only the first derivative of $R_{np}(U)$, and not the second, and second, the positions of the maxima in the first derivative are determined more accu-

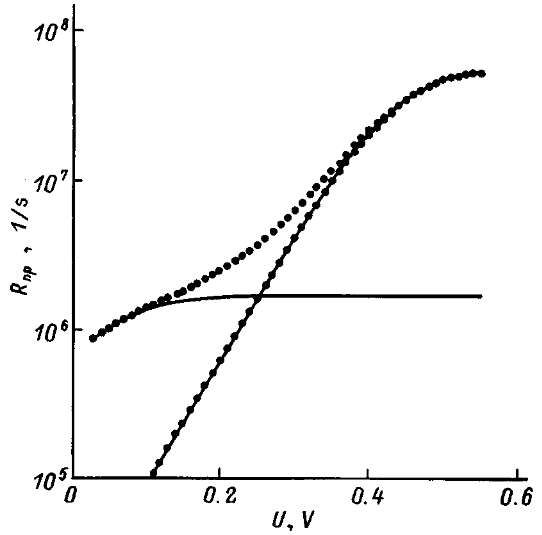

FIG. 1. Separation of the reduced recombination rate into its components ($T=297$ K).

rately than in the second since the numerical ''noise'' in the first derivative is always less than in the second.

THE ($R^2_{np}(U)/\exp(qU/2kT)$) TECHNIQUE

The differential technique described above has one disadvantage: numerical differentiation of the experimental points $\partial R_{np}(U)/\partial U$ leads to an increase in the level of numerical noise in the curve $\partial R_{np}(U)/\partial U$, which complicates the search for U_{0m} substantially. Therefore, we propose another approach. We introduce the function $L(U)$ as follows:

$$L(U)=\frac{R^2_{np}(U)}{\exp\left(\dfrac{qU}{2kT}\right)}. \tag{13}$$

This function has maxima. To find them, we search for extrema:

$$\frac{\partial L(U)}{\partial U}=\frac{\partial}{\partial U}\left(\frac{R^2_{np}(U)}{\exp\left(\dfrac{qU}{2kT}\right)}\right)=\frac{2R_{np}\dfrac{\partial R_{np}}{\partial U}-R^2_{np}\dfrac{q}{2kT}}{\exp\left(\dfrac{qU}{2kT}\right)}=0. \tag{14}$$

Using Eq. (7), we obtain

$$2\frac{q}{2kT}\sum_{m=1}^{s}\frac{\alpha_m\exp\left(\dfrac{qU_{0m}}{2kT}\right)(\zeta^2_m+1)}{\left(2\zeta_m\exp\left(\dfrac{qU_{0m}}{2kT}\right)+\zeta^2_m+1\right)^2}-\frac{q}{2kT}\sum_{j=1}^{s}\frac{\alpha_j\exp\left(\dfrac{qU_{0j}}{2kT}\right)}{2\zeta_j\exp\left(\dfrac{qU_{0j}}{2kT}\right)+\zeta^2_j+1}=0. \tag{15}$$

Keeping track of the summation indices and reducing the left-hand side of Eq. (15) to a common denominator, we obtain

$$\sum_{m=1}^{s}\frac{2\alpha_m\exp\left(\dfrac{qU_{0m}}{2kT}\right)(\zeta^2_m+1)-\alpha_m\exp\left(\dfrac{qU_{0m}}{2kT}\right)\left(2\zeta_m\exp\left(\dfrac{qU_{0m}}{2kT}\right)+\zeta^2_m+1\right)}{\left(2\zeta_m\exp\left(\dfrac{qU_{0m}}{2kT}\right)+\zeta^2_m+1\right)^2}=0. \tag{16}$$

As above, we assume that Eq. (16) is satisfied if each term is equal to zero. Then

$$\zeta^2_m+1-2\zeta_m\exp\left(\frac{qU_{0m}}{2kT}\right)=0, \tag{17}$$

$m=1,2,\dots,s$, which exactly coincides with Eq. (9), and the roots of this quadratic equation in ζ_m are given by formula (10) or (11). However, in the analysis of $L(U)$ the parameter α_m cannot be determined from the amplitude of the maximum or in any other way [see Eq. (13)]. Thus, by analyzing $L(U)$ it is possible only to find ζ_m and then determine E_{tnm} using formula (5).

In comparison with the previous technique, the given technique has the advantage that it does not use numerical differentiation; its disadvantage is that it allows one to determine only the parameter ζ_m.

RESULTS OF ANALYSIS OF THE CURRENT-VOLTAGE CHARACTERISTICS OF Si:Au–p^+–n DIODES AND DISCUSSION

Current–voltage characteristics of a gold-doped silicon p^+-n diode (D-220) were measured at $T=297$ K (24 °C). The reduced recombination rate $R_{np}(U)$ was calculated according to formula (3) for each voltage (Fig. 1). $U_{\mathrm{dif}}(U)$ and $w(U)$ were found in the usual way[11] from the results of capacitance measurements plotted in the same figure. According to formula (4), $R_{np}(U)$ was expanded into its components by the method of successive trial and error (numerical search) of the parameters α_m and ζ_m ($m=1,2$) (each ''ledge'' is described by the pair α_m and ζ_m; see Fig. 1). From the parameter values ζ_1 and ζ_2 the activation energy of the deep levels is calculated using formula (5):

$$E^+_{tn}=0.33+0.01\cdot\ln\frac{c^+_n}{c^0_p};\quad E^-_{tn}=0.53+0.01\cdot\ln\frac{c^0_n}{c^-_p}. \tag{18}$$

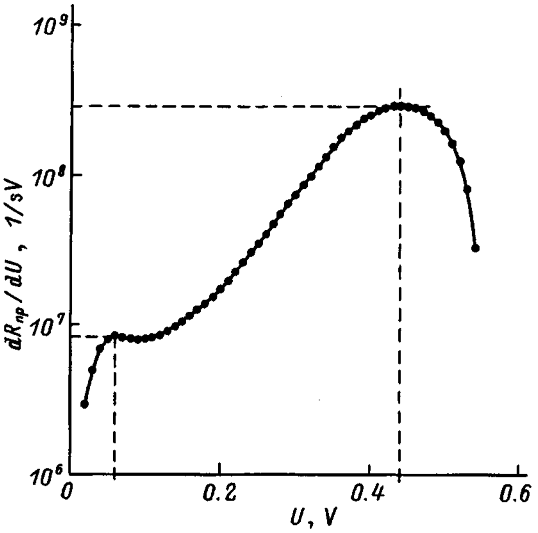

FIG. 2. Derivative of the reduced recombination rate with respect to the voltage ($T=297$ K). Maxima at 0.06 and 0.44 V.

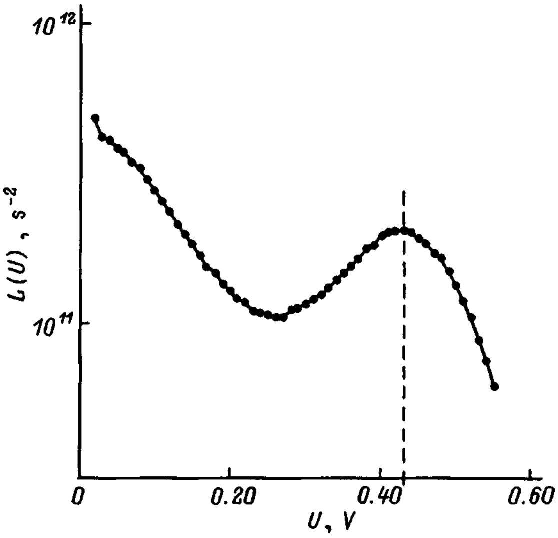

FIG. 3. Reduced recombination rate by the $L(U)$ method. Maximum at 0.43 V.

Since c_n^+, c_p^0, c_n^0, and c_p^- are known [$\ln(c_n^+/c_p^0)\approx 1$, $\ln(c_n^0/c_p^-)\approx 0.4$; Ref. 10], we can determine E_{tn}^+ and E_{tn}^- exactly; however, in general (if the capture coefficients are not known *a priori*) we can only make an approximate estimate. From the expansion of $R_{np}(U)$ into its components we obtain $E_{tn}^+\approx 0.34$ eV and $E_{tn}^-\approx 0.53$ eV, which are in good agreement with the results of other studies.[10] [As is well known,[10] gold impurity in silicon forms two deep levels in the band gap: 1) an acceptor level $E_t=E_c-0.55$ eV; for $T=300$ K $\sigma_n^0=1.7\times 10^{-16}\,\mathrm{cm}^2$ and $\sigma_p^-=1.1\times 10^{-14}\,\mathrm{cm}^2$; and 2) a donor level $E_t=E_v+0.35$ eV; for $T=300$ K $\sigma_n^+=6.3\times 10^{-15}\,\mathrm{cm}^2$ and $\sigma_p^0=2.4\times 10^{-15}\,\mathrm{cm}^2$].

Let us now apply the differential expansion technique to $R_{np}(U)$. The derivative $\partial R_{np}(U)/\partial U$ is plotted in Fig. 2. There are two maxima at $U_{01}=0.06$ V and $U_{02}=0.44$ V. We find ζ_1 and ζ_2 from formula (10) and calculate the activation energy of the deep levels from formula (5):

$$E_{tn}^+=0.33+0.01\ln\frac{c_n^+}{c_p^0};\quad E_{tn}^-=0.52+0.01\cdot\ln\frac{c_n^0}{c_p^-}. \tag{19}$$

The result of processing $R_{np}(U)$ using the second technique $[L(U)]$ is plotted in Fig. 3. The first maximum U_{01} does not show up, but we find $U_{02}=0.43$ V. Using Eqs. (10) and (5), we calculate the activation energy of the deep levels

$$E_{tn}^+=0.33+0.01\cdot\ln\frac{c_n^+}{c_p^0}. \tag{20}$$

It can be seen that results (18), (19), and (20) coincide within 0.01 eV with the results of Ref. 10.

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