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EFFECT OF DEEP IMPURITY LEVELS ON SCHOTTKY BARRIER DIODE CHARACTERISTICS

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Abstract—In the presence of an arbitrary number of deep donor levels volt–ampere and volt–farad characteristics are obtained for the Schottky barrier diode which contains a thin dielectric layer between the metal and the semiconductor. The analysis of these characteristics shows that the deep levels can significantly influence both the capacitance and the rectifying properties of the Schottky diode; the thicker the dielectric layer, the greater the effect of the deep levels upon volt–ampere relationship and the lesser upon volt–farad one. One can determine the parameters of the deep levels from these relationships. The results of the calculation are in agreement with the data of the experiment performed.

1. INTRODUCTION

In recent years attention has often been paid to the part which deep volume impurity levels take in the performance of the Schottky barrier diodes. The physical reason for this phenomenon is the fact that deep levels may play a part in the process of the formation of the semiconductor depletion region. The impact of changes in charge in the depletion region, associated with the deep levels, on the volt-farad (C–V) characteristics as well as the determination of the parameters of the impurity centres have been studied in refs. [1–5]. However the theoretical results obtained until now have been concerned with close metal–semiconductor contacts; at the same time it is known that the physical processes taking place in the contact which contains a dielectric layer between the metal and the semiconductor may be quite different from those involving close contacts [6].

In this paper the effect of the deep donor levels on the rectifying properties as well as on the C–V relationships of the Schottky barrier diodes with an interlayer is considered, also the parameters of these levels are determined. The results of the calculation are compared with the experimental data obtained.

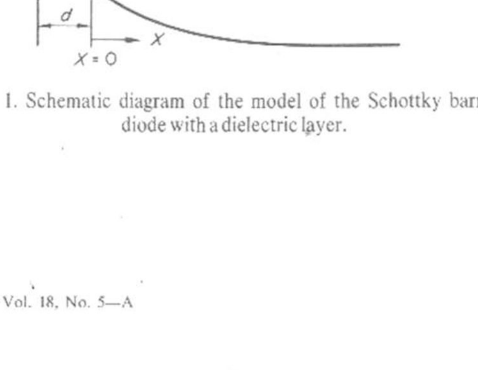

Fig. 1. Schematic diagram of the model of the Schottky barrier diode with a dielectric layer.

It is convenient to describe the rectifying properties of the diodes investigated, the model of which is schematically presented in Fig. 1, with the help of the parameter defining the differential slope of the volt-ampere (I–V) characteristics.

We can introduce this parameter according to [6] in the following form

$$\alpha(V) = \frac{e}{kT}\frac{\mathrm{d}V_2}{\mathrm{d}V} = \begin{cases} \dfrac{\mathrm{d}\ln I}{\mathrm{d}V} & \text{for forward bias} \quad (1) \\[2ex] \dfrac{e}{kT} - \dfrac{\mathrm{d}\ln I}{\mathrm{d}V} & \text{for reverse bias} \quad (2) \end{cases}$$

here V_2 is the voltage drop across the semiconductor, $V = V_1 + V_2$ is the general applied voltage. Relationships (1) and (2) is true for voltages such that $e^{eV_2/kT} \gg e^{-eV_1/kT}$ or $e^{eV_2/kT} \gg e^{-eV_1/kT}$ for forward and reverse bias respectively. If we know the experimental I–V data, then the terms on the right of (1) and (2) allows to determine the function $\alpha(V)$ in the whole range of applied bias.

At sufficiently high frequencies the contact capacitance can be represented as a sum of two series capacitances, one of the dielectric film C_1 and another of the depletion region C_2 [7]:

$$C(V) = \frac{C_1 C_2}{C_1 + C_2} = C_2 \frac{\mathrm{d}V_2}{\mathrm{d}V}. \quad (3)$$

Thus it can be seen from (1), (2) and (3) that both the rectifying and the capacitance properties of the diodes we are dealing with, are characterised with the help of the function $V_2(V)$. We can obtain its explicit form using the condition of continuity of the normal component of the electromagnetic induction vector at the interface[6]:

$$\frac{\epsilon_1}{d} V_1 = \epsilon_2[E(V_2, 0) - E(0, 0)] \quad (4)$$

where $E(V_2, x)$ is the field intensity in the semiconductor, ϵ_1 and ϵ_2 are the permittivities of the dielectric and the semiconductor respectively, V_1 is the voltage drop across the interlayer ($V_1 + V_2 = V$). When writing condition (4) the absence of charged states at the interface is assumed. (The more accurate assumption is that only a part of all surface states can be overcharged; this part satisfies the following inequality

$$\Delta m_s \ll \frac{\epsilon_2}{4\pi e} \Delta E(0)$$

where m_s is the density of surface states). The voltage dependence of the quantity $E(V_2, x)$ expressed in terms of model parameters, can be derived from Poisson's equation

$$\frac{d^2\varphi}{dx^2} = \frac{4\pi e}{\epsilon_2} \rho(x). \quad (5)$$

2. THEORETICAL CALCULATION

Let us assume that the shallow-donor levels in the depletion region of the n-type semiconductor are completely ionised and that there occurs in addition a set of uniform deep donor traps with ionisation potentials E_i where $i = 2, 3, \ldots N$. We regard these levels as energetically non-overlapping, homogeneously distributed in space and also completely ionised in the region where they are localised above the Fermi level (Fig. 1).

If we ignore free carriers then the density of space charge can be expressed by means of the following step function:

$$\rho(x) = e \sum_{k=1}^{i} n_k \quad \text{for} \quad l_{i+1} < x \leq l_i \quad (6)$$

where $i = 1, 2, \ldots, N$; $l_{N+1} = 0$. Here n_k is the concentration of the impurity that gives the k-th level line, the co-ordinates l_i are defined by the following conditions:

$$\varphi(l_i) = E_i - \mu \quad (7)$$

and $\varphi(x)/e$ is the electrostatic potential value relative to the edge of the semiconductor conduction band. Solving Poisson's equation subject to the boundary conditions

$$\varphi(l_1) = 0$$

$$E(V_2, l_1) = -\frac{1}{e}\frac{d\varphi}{dx}\bigg|_{x=l_1} = 0 \quad (8)$$

and using condition (7) when integrating, we find a set of equations for the determination of the quantities l_i as follows:

$$\left.\begin{aligned} \mu - E_i &= \frac{2\pi e^2}{\epsilon_2} \sum_{k=1}^{i} n_k (l_k - l_i)^2, \quad i = 2, 3, \ldots, N-1 \\ \varphi(0) &= \frac{2\pi e^2}{\epsilon_2} \sum_{k=1}^{N} n_k l_k^2. \end{aligned}\right\} \quad (9)$$

Here $\varphi(0) = \varphi_0 - eV_2$, where φ_0 is the potential barrier height at the interface for $V = 0$. It is convenient to represent the solution of this set of algebraic equations in the form of recurrent relations:

$$l_{i+1} = l_i - \frac{r_i + S_i}{\sum_{k=1}^{i} n_k}, \qquad i = 1, 2, \ldots, N;$$

$$l_{N+1} = 0; \quad r_1 = 0; \quad r_i = -\sum_{m=1}^{i-1} n_m \sum_{k=m}^{i-1} \frac{r_k + S_k}{\sum_{j=1}^{k} n_j}; \quad (10)$$

$$S_N^2 = r_N^2 - \sum_{k=1}^{N} n_k \left\{ \sum_{m=1}^{N-1} n_m \sum_{i=m}^{N-1} \left[\frac{r_i + S_i}{\sum_{k=1}^{i} n_k}\right]^2 - \frac{\varphi(0)\epsilon_2}{2\pi e^2} \right\};$$

$$S_i^2 = r_i^2 - \sum_{k=1}^{i} n_k \left\{ \sum_{m=1}^{i-1} n_m \sum_{k=m}^{i-1} \left[\frac{r_k + S_k}{\sum_{j=1}^{k} n_j}\right]^2 - \frac{E_{i-1} - \mu}{2\pi e^2} \right\}, \quad i \neq N.$$

In further investigation of this problem it is necessary to take into account the frequency response of the physical processes taking place in the contact[3–5]; and, just as in ref. [1], we distinguish between two cases:

(1) The case of low frequency. The frequency of recharging of all deep levels is considerably higher than the applied frequency (all deep traps respond to the test frequency $[(dl_i/dV) \neq 0]$.

(2) The case of intermediate frequency. The first K levels respond to the test frequency, and the other $(N-K)$ (lying deeper) do not:

$$\frac{\partial l_i}{\partial V} \neq 0 \quad \text{for} \quad i \leq K$$

$$\frac{\partial l_i}{\partial V} = 0 \quad \text{for} \quad i > K.$$

Now using (1), (4) and (10) it is easy to obtain for $\alpha(V_2)$:

(1) for low frequencies:

$$\alpha = \frac{e}{kT}\left\{1+\frac{ed\epsilon_2}{\epsilon_1}\sum_{j=1}^{N} n_j\left[r_N^2 - \left(\sum_{m=1}^{N-1} n_m \sum_{i=m}^{N-1}\left\{\frac{r_i+S_i}{\sum_{k=1}^{i} n_k}\right\}^2 - \frac{\varphi(0)\epsilon_2}{2\pi e^2}\right)\sum_{k=1}^{N} n_k\right]^{-1/2}\right\}^{-1}. \tag{11}$$

(2) for intermediate frequencies:

$$\alpha = \frac{e}{kT}\left\{1+\frac{ed\epsilon_2}{\epsilon_1}\sum_{j=1}^{k} n_j\left[\sum_{j=1}^{K} n_j \sum_{i=j}^{N-1}\frac{r_i+S_i}{\sum_{k=1}^{i} n_k} + \frac{r_N+S_N}{\sum_{k=1}^{N} n_k}\sum_{j=1}^{k} n_j\right]^{-1}\right\}^{-1}. \tag{12}$$

The relationship $\alpha(V)$ is qualitatively plotted in Fig. 2. The presence of jumps appearing at values $eV_2^i = \varphi_0 - E_i + \mu$ must be emphasized as a main feature of the plotted curve.

The arising of these jumps is caused by the step-like changes in the density of charge $\rho(x=0)$ at values $V_2 = V_2^i$ [according to (6)]. Fermi statistics at $T^\circ = 0$ lead to the sharp shape of these jumps. As the modulating frequency become higher the $\alpha(V)$ extremes become less sharp and disappear when $\omega \gg \tau_i^{-1}$ (τ_i is the relaxation time of ith impurity). The final result of this process yields a dash line in Fig. 2.

As can be seen from expressions (11) and (12), the thicker the oxide film, the greater the effect of the deep levels upon $\alpha(V)$; this effect is equal to zero in the case of the close contact. Thus the dielectric layer being finite, the examination of the $\alpha(V)$ relationships can serve us for the determination of the parameters of the deep traps. The data from the low frequency measurements are more suitable because the point of $\alpha(V)$ jump determines the ionisation potential of the level right away in this case.

The expression for the capacitance of the depletion region is derived from formulae (3), (4) and (10) and for intermediate frequencies can be presented in the following form:

$$\frac{1}{C_2^k} = \frac{1}{C^k} + \frac{1}{C_2^N} \tag{13}$$

where C^k is a constant vs voltage:

$$C^k = \frac{\epsilon_2}{4\pi}\left[\frac{\sum_{m=1}^{k} n_m \sum_{i=m}^{N-1}(l_i - l_{i+1})}{\sum_{m=1}^{K} n_m} - \frac{\sum_{m=1}^{N-1} n_m \sum_{i=m}^{N-1}(l_i - l_{i+1})}{\sum_{m=1}^{N} n_m}\right]^{-1} \tag{14}$$

and C_2^N is the low frequency capacitance:

$$C_2^N = \frac{\epsilon_2}{4\pi}\frac{\sum_{i=1}^{N} n_i}{S_N}. \tag{15}$$

The qualitative course of the relationships $C^{-2}(V)$ and $\Phi = [d(C_2^N)^{-2}/dV]^{-1} = (\epsilon_2 e^2/8\pi)\sum_{k=1}^{i}$ for $E_i < \varphi(0)+\mu < E_{i-1}$ vs applied voltage is pictured in Fig. 3(a) and (b). The solid line shows a low frequency dependence $C^{-2}(V)$ at $d=0$ that is equivalent to $C = C_2^N$. As can be seen, the function $(C_2^N)^{-2}$ is discontinuous at the points eV_2^i determined by the deep-level positions, the magnitude of the discontinuity being dependent on the concentrations of the impurities. Each portion between

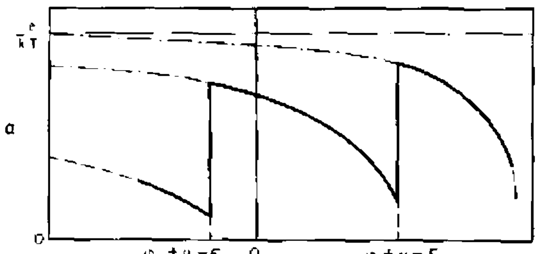

Fig. 2. Qualitative plot of $\alpha = (d\ln J/dV)$ vs V_2 relationship. V_2 is the voltage drop across the depletion region.

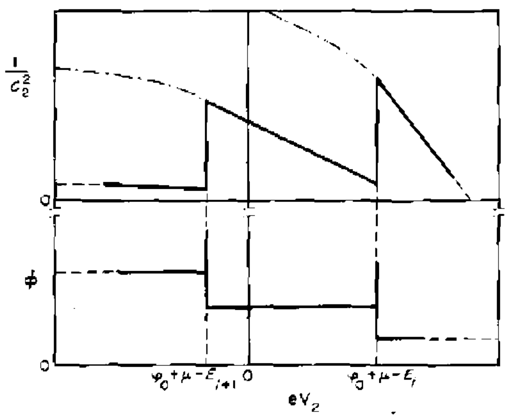

Fig. 3. (a) Qualitative plot of C_2^{-2} vs V_2 relationship. C_2 is the capacitance of the depletion region. (b) Qualitative plot of $\Phi \equiv \left[\frac{d(C_2^N)^{-2}}{dV}\right]^{-1}$ vs V_2 relationship. δ-like peaks widen when $T^\circ \neq 0$.

two subsequent discontinuities is linear, the slopes of these segments decrease when the back bias goes up and are determined by the sum of the concentrations of those impurities which contribute to the Schottky layer capacitance. If a frequency is applied such that ith level 'disengagement' takes place, the discontinuities of the function $[C_2^N(V_2)]^{-2}$ and also the δ-like peaks which separate the steps in $\Phi(V_2)$ both disappear, which leads to matching of the above mentioned portions with each other at the points eV_2^i (dot and dash lines in Fig. 3(a) and (b)).

3. EXPERIMENTAL RESULTS

To check the correctness of the physical ideas which we discuss in this work and to determine the deep-level parameters, the $I-V$ (at low frequency of the applied voltage) and the $C-V$ (at high frequency) characteristics of the Schottky diodes were measured. The diodes were fabricated according to planar technology using GaAs epitaxial structure of $n-n^+$ type. The rectifying contact was made in the following way. A SiO_2 film 0·5 μm thick was applied to the GaAs surface by the ionic-plasma method. Then round openings of 30 μm in diameter were made in the SiO_2 layer. Through these openings nickel was applied electrolytically on the GaAs surface, thus creating Schottky barrier.

The quantity α was determined from the expression $\alpha = (IR)^{-1}$ where I—is the electric current through a diode at a fixed bias and R—is the corresponding differential resistance determined at a frequency 1 kc (the calculation of R requires taking into account semiconductor bulk resistance). For the capacitance measurement the method of Berlin *et al.*[8] was used, the frequency taken equal to 3180 MHz.

A lot of 7 diodes was measured. The measured $C-V$ relationship for a typical diode is presented in Fig. 4. As one can see from this figure, the capacitance becomes a constant at large forward bias, this constant defining the value of C_1, equal to 4·4 pF. The corresponding value of d/ϵ_1 is 14 Å, if we assume that the interlayer is a plane capacitor. The experimental $[C_2(V_2)]^{-2}$ and $\alpha(V_2)$ values are shown in Fig. 5. We see that these dependences have a character analogous to those plotted in Fig. 2 (solid line) and in Fig. 3(a) (dash line) for the case when one deep level is present. One could make an attempt to explain the $C-V$ dependence obtained at high frequency, by the heterogeneous, step-like, distribution of shallow (completely ionised) impurity centers. But it is not the case, since for the step-like distribution of shallow impurities the low-frequency function $\alpha(V)$ must behave like a dash line in Fig. 2, that is in contrast to our experiment. It is also impossible to explain the figured experimental curves by the presence of the electronic surface states at the interface[9], since the $C_2^{-2}(V_2)$ dependence must give a straight line in the last case. (That is why we present the relationships for both the capacitance and the parameter α as the functions of V_2 but not of V. The function $V(V_2)$ can be evaluated from equation (4). The values of the parameters necessary for this purpose can be found out in a manner proposed further). It follows from formulae (11) and (13)–(15) that the expressions for $\alpha(V_2)$ and $C_2^{-2}(V_2)$ for $N = 2$ are: for $\varphi(0) \geq E_2 - \mu$

$$\alpha = \frac{e}{kT}\left\{1 + \frac{d}{\epsilon_1} e^2(n_1 + n_2) \sqrt{\left[\frac{2\pi\epsilon_2}{\varphi(0)(n_1 + n_2) - (E_2 - \mu)n_2}\right]}\right\}^{-1} \quad (16)$$

$$C_2^{-2} = \frac{8\pi}{\epsilon_2 e^2}\left\{\frac{n_2}{n_1 + n_2}\sqrt{\left(\frac{E_2 - \mu}{n_1}\right)} + \sqrt{\left[\frac{\varphi(0)}{n_1 + n_2} - \frac{(E_2 - \mu)n_2}{(n_1 + n_2)^2}\right]}\right\}^2 \quad (17)$$

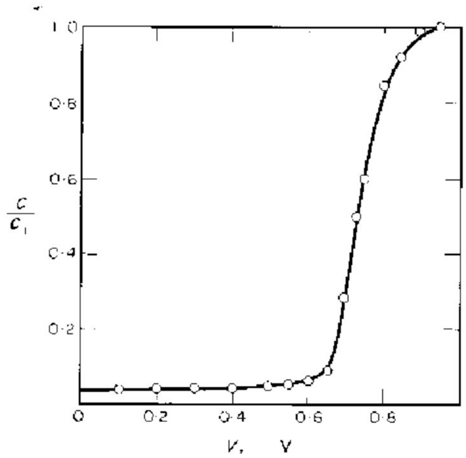

Fig. 4. Experimental curve of C/C_1 vs V relationship. Value of C_1 is 4·4 pF.

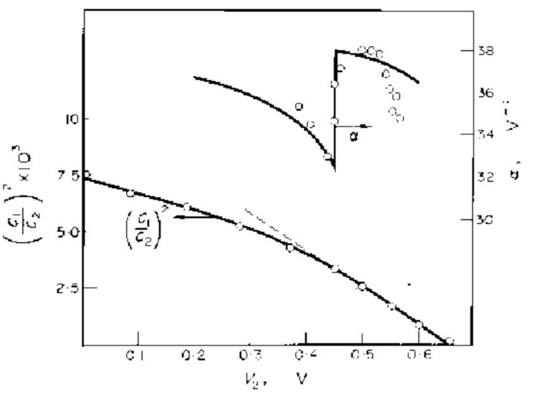

Fig. 5. Experimental and calculated α vs V_2 (16), (18) and $(C_1/C_2)^2$ vs V_2 (17), (19) relationships.

for

$$\varphi(0) < E_2 - \mu$$

$$\alpha = \frac{e}{kT}\left\{1 + \frac{d}{\epsilon_1} e^2 \sqrt{\left[\frac{2\pi\epsilon_2 n_1}{\varphi(0)}\right]}\right\}^{-1} \qquad (18)$$

$$C_2^{-2} = \frac{8\pi}{\epsilon_2 e^2} \frac{\varphi(0)}{n_1}. \qquad (19)$$

The values of the parameters n_1, n_2, $E_2 - \mu_1$, φ_0 were evaluated according to the requirement that the curve obtained from (17) and (19) must coincide with the experimental one at the points where $V_2(V)$ is known, namely $V_2 = 0$, $eV_2 = \varphi_0 - E_2 + \mu$, $eV_2 = \varphi_0$ and the quantity n_1/n_2 can be found out from the extremes of $\alpha(V)$. These values are $n_1 = 2{\cdot}97 \times 10^{15}\,cm^{-3}$, $n_2 = 1{\cdot}04 \times 10^{16}\,cm^{-3}$, $\varphi_0 = 0{\cdot}67\,eV$, $E_2 = 0{\cdot}375\,eV$ ($\mu = 0{\cdot}155$ eV). It is worth mentioning that the value of the potential barrier height is in a good agreement with the values known for GaAs–Ni contacts[11].

The $\alpha(V_2)$ and $[C_2(V_2)]^{-2}$ curves, calculated for the same values of the parameters are shown in Fig. 5 by full lines. We see that the agreement of the theoretical dependence with the experimental one is satisfactory. The discrepancy observed in the region of forward bias of the $\alpha(V_2)$ curve may be a consequence of a current violation of the distribution function of charge carriers[10] or else a consequence of the fact that interface electronic states have been neglected[9].

Thus the deep impurity states significantly influence both the capacitance and the rectifying properties of the Schottky barrier diode with the dielectric interlayer; from the other hand the analysis of these properties can give us the information about the parameters of the deep levels. We wish to emphasize that when the dielectric layer is thick enough the main information about the deep levels is included in the $\alpha(V)$ relationship, since in the limiting case $d \to \infty$ the deep impurities do not affect the contact capacitance which becomes equal to the dielectric film capacitance.

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