Determination of deep-level energy and density profiles in inhomogeneous semiconductors

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(Received 12 March 1973)

A method is proposed for the determination of deep impurity levels and density profiles from C-V measurements and is demonstrated on GaAs Schottky barrier diodes. The technique involves measurements of the time dependence of the bias voltage instead of the barrier capacitance. The spatial distribution of a deep level is observed to exhibit a peak at the boundary between an epitaxial layer and the semi-insulating substrate. This deep center is located 0.8 eV below the conduction band.

When the reverse bias is suddenly incremented, the depletion layer capacitance of a Schottky diode varies gradually with time because of deep-lying impurities. Senechal and Basinski (SB)[1,2] pointed out that this phenomenon is applicable to the determination of energy levels and the density of deep centers in homogeneous semiconductors. Glover[3] extended the SB method to the nonuniform case, but he did not think of a way to obtain density profiles. Zohta and Ohmura[4] suggested that these profiles could be obtained by both the C-V method and the Copeland method.[5] This letter gives a method of measuring the spatial distribution and the energy level of deep centers from C-V measurements alone on Schottky diodes.

The SB model is extended to materials including non-uniform distributions of shallow and deep impurities. The data required in this case are the time variations of the bias voltage which is needed to keep the depletion layer capacitance unchanged during the subsequent transition after the bias is switched from a fixed forward bias V_{Bf} to some negative bias $-V_B(0)$ as shown in Fig. 1.

Let us consider the model of a Schottky barrier formed on semiconductors with $N_S(x)$ compensated shallow donors and $N_T(x)$ deep donors at a level E_T. Taking account of charge states in impurity centers within the depletion region, one can obtain the following expression after double integration of Poisson's equation with the usual boundary condition[6]:

$$V_D - V_B = \tfrac{1}{2}(e/\epsilon)\{W^2 \bar{N}_S(W)$$
$$+ [1 - \exp(-t/\tau)]x_\lambda^2 \bar{N}_T(x_\lambda)\}, \qquad (1)$$

where V_D, V_B, and W are the diffusion potential, the bias voltage, and the width of the depletion region, respectively, and the point $x_\lambda = W - \lambda(W)$ is defined by the crossover of the deep level E_T with the bulk Fermi level E_F. The electronic charge is denoted by e; the dielectric constant, by ϵ. The time constant τ is associated with the transient behavior caused by a deep level. $\bar{N}_S(W)$ and $\bar{N}_T(x_\lambda)$ are the average shallow and deep impurity densities given by

$$\bar{N}_S(W) = (2/W^2) \int_0^W dz \int_z^W N_S(x)\,dx, \qquad (2)$$

and

$$\bar{N}_T(x_\lambda) = (2/x_\lambda^2) \int_0^{x_\lambda} dz \int_z^{x_\lambda} N_T(x)\,dx, \qquad (3)$$

respectively. The high-frequency small-signal depletion layer capacitance for a diode with area S is $C(W) = \epsilon S/W$. One may write, using Eq. (1),

$$\bar{N}_T(x_\lambda)\exp(-t/\tau) = \frac{C^2(W)}{\tfrac{1}{2}\epsilon e S^2\{1 - \lambda(W)[C(W)/\epsilon S]\}^2}\,\Delta V_B(t), \qquad (4)$$

where $\Delta V_B(t) = V_B(t) - V_B(\infty)$; $V_B(t)$ and $V_B(\infty)$ are the values for the bias voltage at a time t after the bias switching and at steady state, respectively. Equation (4)
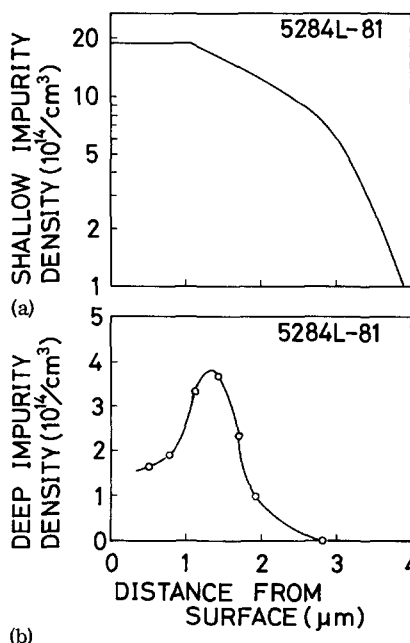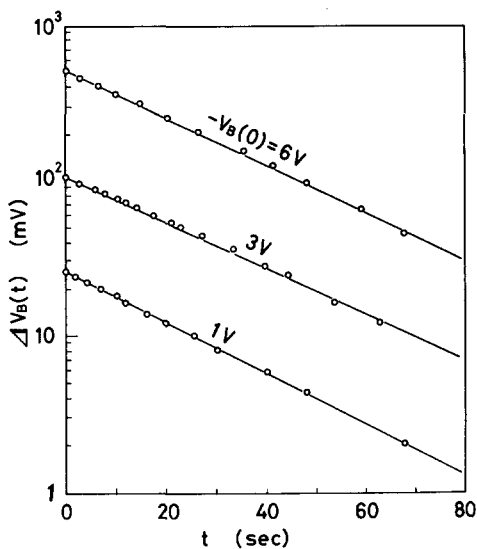

FIG. 1. Temporal sequence of barrier capacitance and bias voltage.

FIG. 2. (a) Profile of shallow impurity density. (b) Profile of deep impurity density.

FIG. 3. Plot of $\Delta V_B(t)$ vs t.

FIG. 4. Temperature dependence of the time constant τ.

indicates that $\Delta V_B(t)$ changes exponentially with time because $C(W)$, $\lambda(W)$, and $\bar{N}_T(x_\lambda)$ are independent of time. Therefore, a semilog plot of $\Delta V_B(t)$ against time gives the time constant τ. The average deep density $\bar{N}_T(x_\lambda)$ is deduced from Eq. (4) by setting $t=0$, if $\Delta V_B(0)$, the total amount of the bias change, and $C(W)$ are measured in addition to the knowledge of $\lambda(W)$. The value for $\lambda(W)$ is determined from the shallow impurity profile, according to[7]

$$\epsilon e^{-2}(E_F - E_T) = \int_{W-\lambda(W)}^{W} dz \int_z^W N_S(x)\, dx. \tag{5}$$

Furthermore, $e^{-1}(E_F - E_T)$ can be obtained as the sum of the diffusion potential and the minimum bias V_{min} that enables a diode to change its capacity. If $E_C - E_F$ is known, it is also estimated from the temperature dependence of the time constant,[8] $\tau = A \exp[(E_C - E_T)/kT]$, where A is a slowly varying function of temperature T, k is Boltsmann's constant, and E_C is the energy level of the conduction band edge.

Equation (3) leads to the following expression:

$$N_T(x_\lambda) = \bar{N}_T(x_\lambda) + \tfrac{1}{2}x_\lambda \frac{d\bar{N}_T(x_\lambda)}{dx_\lambda}. \tag{6}$$

Thus, one can determine the deep impurity profile from a set of average deep densities which are known through the process stated above. The similar expression between $N_S(W)$ and $\bar{N}_S(W)$ is deduced from Eq. (2), which is used to determine the shallow impurity profile. Note that the average shallow impurity density can be obtained if the capacitance is measured immediately after the bias is applied.

The important feature of this method is that the spatial region of interest in the junction does not change by monitoring of V_B for fixed C. In the other regime,[1-3] in some cases, the changing volume of the depletion layer can cause additional difficulties.

We have experimented on Schottky diodes fabricated from oxygen-doped n-type bulk GaAs wafers to confirm our method. The result is that $\bar{N}_T = 2 \times 10^{16}$ cm^{-3} and $E_C - E_T = 0.86$ eV, which is in good agreement with the result that $\bar{N}_T = 2 \times 10^{16}$ cm^{-3} and $E_C - E_T = 0.83$ eV, obtained using the SB method. The shallow impurity density of this sample is 4.5×10^{15} cm^{-3}.
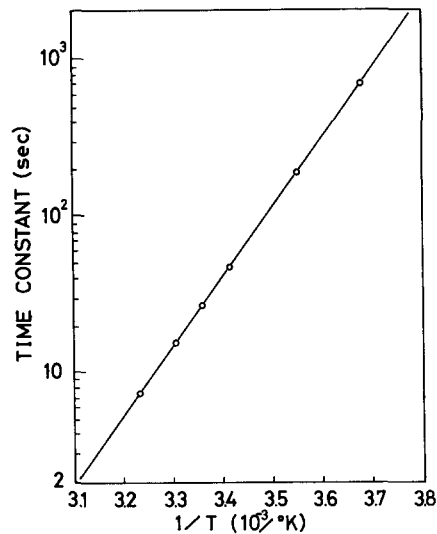
Our method has also been applied to determine the profile and the level of deep centers existing at the tail of n-type epitaxial GaAs layers deposited on (100) Cr-doped semi-insulating substrates in an $AsCl_3/Ga/H_2$ system. The experiment was performed at room temperature. The shallow impurity profile of a sample is shown in Fig. 2(a). Figure 3 shows plots of $\Delta V_B(t)$ vs t for three values of the initial bias $-V_B(0)$. One can observe that they are straight lines following the relation of Eq. (4). For initial biases higher than 9 V, the lines are curved. This deviation from theory is explained in terms of electron capture by the trap as the current increases due to impact ionization.[9] The time constant estimated from the slopes of these lines is 29 ± 2 sec. Figure 2(b) illustrates the obtained deep impurity profile. It shows a peak at the position where the shallow impurity density begins to fall off. It is not clear whether this kind of peak is common or not, concerning the epitaxial GaAs layer on the semi-insulating substrate. The activation energy obtained from V_D and V_{min} is 0.84 ± 0.05 eV. It agrees well with 0.88 ± 0.04 eV, estimated from the temperature dependence of the time constant, which is shown in Fig. 4. This level may be attributed to oxygen, but further study would be necessary to clarify this point.

In conclusion, a simple method has been presented to determine deep impurity levels and profiles which are applicable even when the shallow impurity density is not uniform and is considerably high as compared with the deep density. This method can provide detailed information on the deep center with high precision.

[1]R. R. Senechal and J. Basinski, J. Appl. Phys. **39**, 3723 (1968).
[2]R. R. Senechal and J. Basinski, J. Appl. Phys. **39**, 4581 (1968).
[3]G. H. Glover, IEEE Trans. Electron Devices **ED-19**, 138 (1972).
[4]Y. Zohta and Y. Ohmura, Appl. Phys. Lett. **21**, 117 (1972).
[5]J. A. Copeland, IEEE Trans. Electron Devices **ED-16**, 445 (1969).
[6]For the deep acceptors, $\bar{N}_S$ and N_S with arguments x and W are replaced by $\bar{N}_S - \bar{N}_T$ and $N_S - N_T$, respectively, in Eqs. (1), (2), and (5). Other part stays unchanged.
[7]When $W \gg \lambda(W)$ holds, Eq. (5) reduces to $\Lambda(W) \approx [2\epsilon(E_F - E_T)/e^2 N_S(W)]^{1/2}$.
[8]C. T. Sah, L. Forbes, L. L. Rosier, and A. F. Tasch, Jr., Solid-State Electron. **13**, 759 (1970).
[9]R. Williams, J. Appl. Phys. **37**, 3411 (1966).