THEORETICAL INVESTIGATION OF THE C-V RELATIONSHIP FOR AN AMORPHOUS SILICON p - n JUNCTION

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Abstract—The use of capacitance-voltage measurement to probe the continuous gap state distribution of hydrogenated amorphous silicon is reconsidered. Since the capacitance is measured by a small a.c. voltage, whereas the data is plotted against d.c. voltage, care must be taken in extracting the gap state density from the slope of the capacitance-voltage curve. It is found that under large reverse bias, the $1/C^2$ - V curve of an a-Si:H p ⁺- n junction shows a linear relation, similar to a crystal junction, and that the density obtained is the total gap state charge density.

1. INTRODUCTION

Since the first introduction of junction capacitance-voltage (C - V) measurements in characterizing the semiconductor gap states[1], the capacitance method has been developed to many different variations such as C - T , C - ω , C - T - ω and transient measurements[2], where T , ω are temperature and frequency, respectively. These methods were applied to crystalline as well as to amorphous junctions to obtain information about the density of the shallow impurity states or gap state distribution. However, due to the presence of a continuous gap state distribution, the theoretical analysis for an amorphous junction is far more difficult than the crystal case.

Among these studies, analysis of the C - V measurement was almost always based on the results of Roberts and Crowell[3], which required all the deep states to respond to the measuring a.c. signal. This assumption is questionable for hydrogenated amorphous silicon (a-Si:H) junction, since no matter how low the frequency is, say 0.1 Hz, there are still some states which cannot respond[4]. Lang *et al.*[5] have noted this difference, namely that the capacitance is the measure of a specific width within the depletion region depending on the frequency of the a.c. measuring voltage while the total depletion width is determined by the d.c. bias voltage. This difference suggests that the gap state density obtained from the C - V curve is determined by those states that can follow the bias voltage. However, to our knowledge, no explicit formulation has been derived. In this paper, we will present a detailed analysis of the C - V measurement of an a-Si:H p ⁺- n junction and show that the deep levels could be probed by varying the bias voltage, not the a.c. measuring voltage.

In order to derive the C - V relation, the charge distribution in the depletion region must be first determined. This distribution, $\rho(x)$, is determined by the density of the gap states, $N(E)$, and the electron

occupation probability, $f(E, x)$, at different biases and can be expressed as:

$$\rho(x) = \int_{E_v}^{E_c} N(E)[f(E, x) - f_0(E, x)] dE, \quad (1)$$

where $f_0(E, x)$ is the occupation probability at equilibrium, x is the position. Although the density of gap states is strongly affected by the preparation conditions and is not known in all cases, the occupation probability can still be determined. In the following, we shall first use the Shockley-Read-Hall (SRH) recombination model[6,7] to determine the electron occupation probability $f(E, x)$ of the same deep states in three different conditions that will be present in a reverse biased junction. Then the carrier transport equations are investigated self-consistently to determine how these three conditions are met in the depletion region. With this occupation probability and the assumption of a uniform media, the charge distribution can be obtained.

2. THEORY

According to the SRH model, the electron occupation probability of an gap state with energy level, E , can be written as[8]:

$$f(E, x) = \frac{n + b\bar{p}}{n + \bar{n} + b(p + \bar{p})}, \quad (2)$$

where p and n are the free hole and free electron concentration at position x , respectively, which also represent the hole and electron capture rate of the state at E . $\bar{p}$ and $\bar{n}$ for a donor-type gap state are given by:

$$\bar{n} = \frac{N_c}{g} \exp\left(\frac{E - E_c}{kT}\right)$$

$$\bar{p} = gN_v \exp\left(\frac{E_v - E}{kT}\right)$$

which are related to the emission rate of the state E , where g is the degeneracy factor, E_c and E_v the respective conduction and valence band mobility edges, N_c and N_v the corresponding effective densities of states, $b = \sigma_p v_p / \sigma_n v_n$, where σ_p (σ_n) and v_p (v_n) are the hole (electron) capture cross-section and the thermal velocity, respectively. For an acceptor-type gap state, the g factors in the formula for $\bar{n}$ and $\bar{p}$ are replaced by $1/g$. Since the emission rate of a gap state is dependent on its energy, a special energy, E'_i , at which the state has equal electron and hole emission rate, i.e. $\bar{n} = b\bar{p}$, can be defined:

$$E'_i = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln \left(\frac{g^2 b N_v}{N_c} \right), \quad (3)$$

which is close to the intrinsic Fermi level, E_i , differing only by a small quantity, $kT/2 \ln(g^2 b)$. Now we shall consider $f(E, x)$ at three different locations inside the depletion region in a reverse-biased pn junction. Typically, under reverse bias, the hole quasi-Fermi level E_{fp} is situated always above the electron quasi-Fermi level E_{fn} . Figures 1 (a), (b) and (c) show the relative positions of E_{fn} , E_{fp} and E'_i in the gap. When E_{fn} and E_{fp} are all above (below) E'_i , as shown in Fig. 1(a) (Fig. 1b), $f(E, x)$ can be estimated from eqn (2) which turns out to approximately equal to 1 for E less than E_{fn} (E_{fp}). Thus, in these two cases, the electron occupation probability of the gap state is

determined by the majority carrier quasi-Fermi level which depends on the external bias. On the other hand, when E'_i is located in between E_{fn} and E_{fp} (Fig. 1c), $f(E, x)$ is determined by E'_i which is solely dependent on the material properties and independent of the external bias. This suggests that, when the free carrier density is sufficiently small, the occupation probability of the gap state is determined by the emission rate of the states and independent of the applied bias[9].

Next, we shall use the continuity equation to derive the variation of E_{fn} and E_{fp} , in a reverse biased p^+-n junction. Considering both diffusion and drift currents, the electron current density can be written as[10]:

$$J_n = n\mu_n \nabla E_{fn},$$

where μ_n is the electron mobility and n is the electron concentration n given by:

$$n = N_c \exp[-(E_c - E_{fn})/kT].$$

This equation can be integrated from the edge of the depletion layer $y = W$ to x (Fig. 2a), i.e.

$$\frac{\Delta E_{fn}}{kT} = \ln \left(1 + \int_W^x \frac{J_n}{n(W)\mu_n kT} \exp \left(\frac{\Delta E_c(y)}{kT} \right) dy \right), \quad (4)$$

where $\Delta E_{fn} = E_{fn}(x) - E_{fn}(W)$ and $\Delta E_c(y) = E_c(y) - E_c(W)$. In Fig. 2(a), a linear variation of the mobility edges E_c and E_v has been used. This is only for illustration purposes and irrelevant to the following discussions. The electron current density $J_n(x)$ in eqn (4) is not constant due to the generation process in the reverse-biased junction and can be obtained from the continuity equation:

$$J_n(x) = J_n(W) - \int_W^x eG(y) dy, \quad (5)$$

where $G(y)$ (>0) is the net electron-hole generation rate in the depletion region.

According to eqn (4), ΔE_{fn} can be approximated by:

$$\frac{\Delta E_{fn}}{kT} = \begin{cases} 0 & \text{if } A < 1 \\ \ln(A) & \text{if } A > 1 \end{cases}, \quad (6)$$

where

$$A \equiv \int_W^x \frac{J_n}{n(W)\mu_n kT} \exp \left(\frac{\Delta E_c(y)}{kT} \right) dy. \quad (7)$$

Although, it is difficult to carry out the integration analytically, however, we can simplify it by first considering a crystal junction under the same conditions. In that case, eqns (4), (6) and (7) can still be applied because up to now we do not restrict the derivation to crystal or amorphous junction. Then, $\Delta E_c(x)$ can be obtained based on the depletion approximation:

$$\Delta E_c(x)/kT = [(x - W)/l]^2/2,$$

where $l [\equiv \sqrt{(\epsilon kT)/(q^2 N_D)}]$ is the Debye length. Since the most important contribution to the eqn (7) comes

Fig. 1. Three different conditions that will present in a reverse biased junction. The electron and hole capture rates are significant in (a) and (b), respectively, and the emission rate is dominant in (c). The electron occupation probability, $f(E)$, in each case are also shown.

Fig. 2. A schematic diagram of (a) the energy diagram and (b) the charge distribution of a $p^+ - n$ junction. The coordinates used in the text are also marked. The charge distribution was constant within $a \leq x \leq b$ and the hatched area indicated its change due to the a.c. signal.

from the position around x and $J_n(x)$ is a slowly varying function as compared to $\exp(\Delta E_c/kT)$, the integration can be approximated by multiplying the integrand at x by a distance $l^2/(W-x)$ at which the integrand reduces to 36.8% (e^{-1}) of the maximum value, i.e.

$$A \approx \frac{J_n l^2}{n(W)(W-x)\mu_n kT} \exp\left(\frac{\Delta E_c(x)}{kT}\right). \quad (8)$$

Let A equal to 1 at $y = y_0$, i.e.

$$\Delta E_c(y_0) \equiv kT \ln\left(\frac{n(W)(W-y_0)\mu_n kT}{J_n l^2}\right), \quad (9)$$

and substitute this back into eqns (6) and (7), ΔE_{fn} can be approximated by:

$$\Delta E_{fn} \approx \begin{cases} 0 & \text{if } x > y_0 \\ \Delta E_c(x) - \Delta E_c(y_0) + kT \ln\left(\frac{J_n(x)(W-y_0)}{J_n(y_0)(W-x)}\right) & \text{if } x < y_0 \end{cases} \quad (10)$$

i.e. E_{fn} holds constant for x larger than y_0 and almost parallel to E_c for x smaller than y_0 , as shown schematically in Fig. 2(a). This result, however, is solely dependent on the relative change of ΔE_c and J_n and is irrelevant to whether a crystal or amorphous

junction is involved. Next, we should assume that the approximation can be applied to the amorphous junction and make a self-consistent check later.

Based on the above approximation, the magnitude of $\Delta E_c(y_0)$ can be calculated. Assume the following parameters: $J_n = 10 \text{ nA/cm}^2$, $\sigma_n = 10^{-7} (\Omega \cdot \text{cm})^{-1}$, and $l = 1000 \text{ \AA}$,

$$\Delta E_c(y_0) = 14kT$$

The position of E'_i which is defined in eqn (3) and treated as the intrinsic Fermi level can be roughly estimated from the activation energy ($\sim 1.0 \text{ eV}$) of those lightly boron-doped a-Si:H that show the minimum dark conductivity. The separation between E'_i and E_F of n -type a-Si:H can be readily obtained from its activation energy. The typical value for a n layer doped with 1 ppm PH_3 ($\sigma_D \approx 10^{-7} (\Omega \cdot \text{cm})^{-1}$) is approximately $10kT$. A similar discussion can be applied to E_{tp} . The resultant relative position between E_{fn} , E_{tp} and E'_i is shown in Fig. 2(a), and the crossover points between E'_i and E_{tp} , E'_i and E_{fn} are defined to be a and b , respectively. Following previous discussions, the electron occupation probability, $f(E, x)$, is determined by E_{tp} , E'_i and E_{fn} within $x \leq a$, $a \leq x \leq b$, and $b \leq x \leq W$, respectively.

The most important thing should be noted here is that in the region between a and b , $f(E, x)$ is determined by E'_i and independent of the position. If the gap state density is uniform, the space charge density in this region is also constant. Thus it is possible to define a density called "net gap state density" N in this region, i.e. in the zero temperature approximation:

$$N = \int_{E'_i}^{E_F} N(E) dE,$$

where E_F is the equilibrium Fermi-level position.

In the other two regions, however, no such simple results can be found, as $f(E, x)$ is determined by E_{fn} and E_{tp} , respectively. It is then natural to separate the depletion region into three parts in the following discussions. Figure 2(b) shows schematically the charge distribution (—) in each region under a bias V . Several properties of these regions should be noted. First, the electrostatic potential difference between $x = 0$ and $x = a$ (region 1) is equal to $[E'_i(0) - E_{tp}(0)]/e$ ($\equiv V_p$) and holds constant at all

biases. Similarly, the difference between $x = b$ and $x = W$ (region 3), $[E_{fn}(W) - E'_i(W)]/e$ ($\equiv V_n$) also holds constant. Since the built-in potential, V_{bi} , is equal to $V_n + V_p$, we conclude that all the external bias, V is applied over the constant charge region

from $x = a$ to $x = b$ (region 2), i.e.

$$V = \frac{qN}{2\epsilon} (b-a)^2 + \frac{d\phi}{dx} \Big|_b (b-a), \quad (11)$$

where N is the gap state density, ϕ the electrostatic potential in the depletion layer. Another point should be noted here that the charge stored in region 3, Q_3 should be the same at all voltage biases, since $d\phi/dx$ is vanished at $x = W$. This means that $(d\phi/dx)|_b (= Q_3/\epsilon)$ in eqn (11) is also a constant.

In order to derive the C - V relation, we need to know the change of total charge under a small a.c. signal. Starting from Poisson's equation, $d^2\phi/dx^2 = -\rho(x)/\epsilon$, multiply both sides by $2(d\phi/dx)$ and integrate from $x = a$ to 0, the following equation is obtained:

$$\left(\frac{d\phi}{dx}\right)^2 \Big|_0 - \left(\frac{d\phi}{dx}\right)^2 \Big|_a = \frac{-2}{\epsilon} \int_{\phi(a)}^{\phi(0)-V_p} \rho(\phi) d\phi$$

The values of $\epsilon(d\phi/dx)$ at $x = 0$ and a correspond to the total charge Q_1 and $Q_2 + Q_3$, respectively, where Q_1 is the total space charge, Q_2 and Q_3 are the charges stored in region 2 and 3, respectively. The integral in the right hand side has the order of Q^2 and we can define an equivalent charge, Q_{1eq} , such that:

$$Q_{1eq}^2 = Q_1^2 - (Q_2 + Q_3)^2 = \frac{-2}{\epsilon} \int_{\phi(a)}^{\phi(0)-V_p} \rho(\phi) d\phi. \quad (12)$$

During the C - V measurement, however, the situation is more complex as some deeper states can not respond to the a.c. signal. The possible charge distribution after bias increases to $V + dV$ is shown in Fig. 2(b) (---). From eqn (12), the variations of total charge can be separated into two parts, one due to Q_{1eq} and the other due to $Q_2 + Q_3$. As bias is increased, the second one will eventually dominate and ΔQ_1 can be approximated by:

$$\Delta Q_1 \approx \Delta(Q_2 + Q_3).$$

The change in voltage can be obtained by rewritten eqn (11):

$$V = \frac{qN}{2\epsilon} [(b-a+\bar{x}_3)^2 - \bar{x}_3^2],$$

where $\bar{x}_3 [= Q_3/(qN)]$ is an equivalent width of region 3. The second term can be neglected at large reverse bias as compared to the first one. Since the emission rate for deep states depends exponentially on their activation energy, a new level E_j could be defined (Fig. 2a) such that all the states with energies above E_j and thus with very fast emission rates can respond to the a.c. measuring signal. E_j intersects E_{in} at x_0 in region 3. If the charge stored in the rear part of region 3 ($x_0 \leq x \leq W$) is defined as Q_4 and the charge density at x_0 is $N(x_0)$ then the capacitance C measured using a.c. signal is given by:

$$C = \frac{\epsilon}{x_0 + \bar{x}_4}, \quad (13)$$

where $\bar{x}_4 = Q_4/[qN(x_0)]$. Substituting back into eqn (11), we obtain:

$$V \approx \frac{\epsilon q N}{2} \left[\left(\frac{1}{C} + \frac{1}{C_0} \right)^2 \right], \quad (14)$$

where $1/C_0 [= ((b-a+\bar{x}_3) - (x_0+\bar{x}_4))/\epsilon]$. For sufficiently large bias, $1/C \gg 1/C_0$, the $1/C^2$ - V curve of an amorphous junction shows a linear dependence on bias voltage and is quite similar to a crystal junction.

Based on these results we can check the previous assumption that the electron current density J_n changes slower than the factor $\exp(\Delta E_c/kT)$. From the SRH model the recombination rate, $R(E)$, is expressed as:

$$R(E) = N_1(E) \mu_p \sigma_p \frac{(pn - n_i^2)}{n + \bar{n} + b(p + \bar{p})}.$$

The denominator is smallest within $a \leq x \leq b$ and independent of x . Therefore the generation rate, $G(x)$, in eqn (5) can be regarded as constant within $a \leq x \leq b$. This means that J_n depends, at most, linearly on x and should rise much slower than $\exp(\Delta E_c/kT)$ which depends exponentially on x^2 .

At this stage, the influence of measuring frequency on the capacitance is clear. The variation of the measuring frequency will change the parameter x_0 in eqn (13) and thus affect the measured capacitance. However, at large reverse bias, $1/C_0$ becomes so small the linear $1/C^2$ - V curve is preserved. As defined before, the density N obtained is independent of the a.c. frequency.

Finally, we should discuss the effects of dangling bonds which have two charged states and are not accounted for by the SRH model. Although the presence of two charged states render the SRH formulation inapplicable, the basic physical concept should exist. No matter what the nature of the gap state is, if the free carrier density is small enough to make the emission rate dominant, the electron occupation probability should be determined by the relative magnitudes of the electron and hole emission rate. This will make $f(E)$ independent of x and ensure the existence of a constant charge region.

3. EXPERIMENTS

The a-Si:H $p^+ - n - n^+$ junctions were fabricated in a conventional capacitively coupled glow discharge system. Figure 3 shows the device structure. The substrate was precoated with 1800 Å indium tin oxide (ITO) and 200 Å tin oxide. The gas phase doping concentration was 0.3% for both p^+ and n^+ layer, with 1 ppm PH_3 doping for the n layer. During the deposition, the chamber pressure, substrate temperature, and rf power were kept at 0.5 Torr, 250°C, and 1 W, respectively. The thickness of each layer was 500 Å, 1.2 μm, and 500 Å. After the deposition, Al was evaporated through a metal mask. The final device has an area of $3 \times 10^{-2} \text{ cm}^2$.

Fig. 3. The device structure of the $p^+ - n$ junction used for the capacitance voltage measurement.

Fig. 4. The $1/C^2$ vs bias voltage V of an $a - \text{Si:H } p^+ - n$ junction with gas phase ratio of 1 ppm PH_3/SiH_4 in the n layer.

Table 1. Summary of the net gap state density, N , for different PH_3 doping in the n layer

PH_3/SiH_4 (ppm)	N ($\times 10^{16} \text{ cm}^{-3}$)	Density of state ($\times 10^{17} \text{ cm}^{-3} \text{ eV}^{-1}$)
1	1.8	0.6
10	2.5	1.0
100	4.9	2.5

4. RESULTS

Figure 4 shows the $1/C^2$ vs bias voltage curve of an $a - \text{Si:H } p^+ - n$ junction, with 1 ppm PH_3 doped in the n layer, measured at 10 K, 100 K and 1 MHz, respectively. The d.c. biases are changed slowly at approximately 0.25 V/min. As predicted from the theory, the slopes of the curves are independent of the a.c. measuring frequencies, since the measured charge

density is determined by the d.c. bias voltage not those responded to the a.c. voltage. From the slope of the linear part of the curve, we obtain a net gap state density, N , of $1.8 \times 10^{16} \text{ cm}^{-3}$ and the slopes were almost parallel for the three frequencies. Considering the difference between E'_i and E_F being $\sim 0.3 \text{ eV}$ (estimating from the dark conductivity ratio), the density of state near E'_i is approximately $6 \times 10^{16} \text{ cm}^{-3} \text{ eV}^{-1}$ and is comparable to the results from DLTS. The capacitance decreases as the frequency is increased. This is because at higher frequency the E'_i level became shallower and the distance x_n will be increased to result in a lower capacitance. However, at low bias, the $1/C^2 - V$ curve deviates from the linear relation since the assumption of eqn (14) is violated. The net gap state density for the samples of different PH_3 doping in the n layers are summarized in Table 1. The densities were around 10^{16} cm^{-3} and increased as doping increased. Since the dark conductivity was approximately $10^{-4} (\Omega - \text{cm})^{-1}$ for doping higher than 40 ppm, the density of 100 ppm doping is influenced by the free electron density.

5. CONCLUSIONS

Based on the SHR recombination model and carrier transport equation, we have reconsidered the results of $C - V$ measurements and find that the linear relation between $1/C^2$ and V is also preserved as in the crystalline case. Also the densities obtained from the slope are for those states situated between the equilibrium and the intrinsic Fermi-levels, not those responded to the a.c. signal.

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