Current-voltage characteristics and interface state density of GaAs Schottky barrier

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A density distribution of the interface states in GaAs Schottky barrier was derived for the first time from observed nonideal I-V characteristics of a GaAs Schottky barrier with an oxidized interface. With increasing forward bias voltage, the ideality factor increases and then decreases after passing a maximum. Fermi level of the interface states shifts with the applied bias in the interfacial layer model adopted for the analysis. The obtained energy level of the interface states is in agreement with a previously reported value. However, the absolute magnitude of the state density is quite small compared with that obtained from the weak dependence of the barrier height on metal work functions. Implications of this result are discussed.

There have been extensive studies on interface or surface states of compound semiconductors.[1] However, there still remain unsettled questions. The questions especially arose from the fact that the Schottky barrier height of compound semiconductors such as GaAs is weakly dependent on a variation of the work function of a metal constituting the electrode. This weak dependence is called the surface Fermi level pinning. The interfacial layer model[2] was devised to explain this surface Fermi level pinning. A thin insulating layer is present between the semiconductor and the electrode metal, and interface states of the semiconductor are occupied by electrons to the Fermi level which is different from the neutral level. The occupation of the interface states produces a space charge, which in turn induces a potential difference within the interfacial layer and reduces the effect of work function on the barrier height.

The interfacial layer model was originally developed for an equilibrium condition without applied voltage, where the Fermi level is constant throughout the sample. We extended this interfacial layer model to analyze nonideal I-V characteristics of a-Si Schottky barrier.[3] When a forward bias voltage is applied, a difference arises between the metal Fermi level E_{Fm} and the semiconductor Fermi level E_{Fs}. Fermi level E_{Fi} in the interface states is located between these two Fermi levels. Additional space charge is produced by this shift of E_{Fi} from its equilibrium position and the I-V characteristics become nonideal. For a-Si and c-Si Schottky barriers, a constant density of interface states with respect to energy level was enough to successfully explain observed nonideal I-V characteristics.[3,4] In this report, nonideal I-V characteristics of the GaAs Schottky barrier are analyzed by the interfacial layer model to obtain the density distribution of interface states.

The GaAs wafers used to fabricated Schottky barriers were HB-grown n-type (100) wafers with carrier concentration 1×10^{17} cm^{-3}. Two kinds of Schottky barrier were prepared. Sample A was treated by ultrasonic washing, HCl rinsing, and deionized water cleaning to remove native oxide just prior to Al evaporation. The surface of sample B was thermally oxidized at 500 °C for 5 min in a dry oxygen atmosphere after the removal of native oxide as was done for sample A, then Au was evaporated onto the surface of sample B as the Schottky contact.

For these samples, forward I-V characteristics were precisely measured and the ideality factor n was obtained as a function of the applied voltage V. The ideality factor is defined as $d(\ln I)/dV=q/nkT$, where q is the electron charge and kT is the thermal energy. The behavior of n is quite different between samples A and B as shown in Fig. 1. For sample A, n is nearly unity up to about 0.3 V and then increases with increasing voltage. For sample B, n increases to more than three with increasing voltage up to 0.24 V, then it decreases. While such a voltage dependence in sample B has not been observed in either a-Si or c-Si Schottky barrier, it is more or less observed in the GaAs Schottky barrier with oxidized interface. Therefore, the cause of this strange behavior is considered to be due to characteristics of interface states particular to the GaAs Schottky barrier. It has been reported[5] that the interface

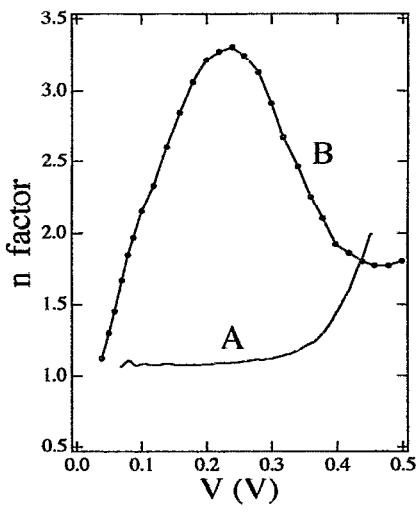

FIG. 1. Ideality factor n vs forward applied voltage V for samples A and B GaAs Schottky barrier with different treatment of interfacial layer.

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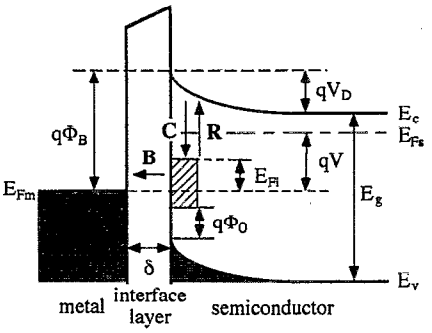

FIG. 2. Energy band diagram of the interfacial layer model of the Schottky barrier under forward bias illustrating electron transitions. The shaded area indicates the occupied interface states constituting space charge.

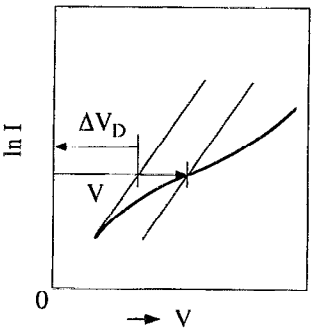

FIG. 3. Observed I-V characteristics and two ideal $n=1$ slopes illustrating how to determine $(V+\Delta V_D)$ value for each applied voltage.

states density of the GaAs Schottky barrier has two peaks over a background in the energy distribution in contrast to that of Si Schottky barrier. Hence, there may be correlations between this strange behavior and the energy distribution of the interface states in GaAs.

Electrons in the interface states communicate with the conduction band of the semiconductor by capture and release processes and also with the metal by tunneling. When a bias voltage V is applied, the occupation of the interface states by electrons can be represented by the Fermi level E_{Fi} of the interface states. Figure 2 illustrates these electron transitions to and from the interface states and E_{Fi} under forward bias in an energy band diagram of the Schottky barrier. Depending on the relative magnitude of these communication possibilities, E_{Fi} is equal to or less than $E_{Fs}=qV$. Here, the metal Fermi level, E_{Fm}, is taken as the zero energy. Thickness of the insulating interfacial layer δ is much smaller than the depletion layer thickness x_D. Hence the change $\Delta\phi_B$ in the barrier height ϕ_B from its zero-bias value ϕ_B^0 produced by the space charge due to occupation of the interface states up to E_{Fi} is given by[3]

$$\Delta\phi_B=\phi_B-\phi_B^0=(1-\gamma)(E_{Fi}/q), \tag{1}$$

where

$$\gamma=1/[1+(\delta q^2 D_s/\epsilon_i)], \tag{2}$$

D_s is the density of interface states $(\mathrm{cm}^2\ \mathrm{eV})^{-1}$, and ϵ_i is the dielectric constant of the insulator. The change ΔV_D is the diffusion potential V_D due to the applied bias V is[3]

$$\Delta V_D=\Delta\phi_B-V. \tag{3}$$

The electron capture probability by the interface states from the conduction band is given by $C=C_0\exp[-q(\phi_B-V)/kT]$, where C_0 is a constant. The thermal release probability of electrons from the interface states is given by $R=\nu\exp[-(q\phi_B-E)/kT]$, where ν is a constant and E is the energy of electrons in the interface states. The tunneling probability of electrons in the interface states into the metal is nearly independent of electron energy and is given by B. The occupation probability f of the interface states by electron is $f=C/(C+R+B)$. In a steady state, it is possible to define E_{Fi} as the energy level where $f=1/2$ and $C=R+B$, since B is a perturbation that is nearly constant. Therefore, the variation of E_{Fi} with applied voltage is obtained by differentiating the relation $C=R+B$,

$$(1/q)(dE_{Fi}/dV)=1/[1-\gamma(B/C)]. \tag{4}$$

The current I of the Schottky barrier is given by[3]

$$I=I_0\exp(-q\phi_B^0/kT)\exp(-q\Delta V_D/kT), \tag{5}$$

where I_0 is a constant. From Eqs. (1), (3), and (4), it becomes

$$dV_D/dV=(1-\gamma)(1/q)(dE_{Fi}/dV)-1. \tag{6}$$

The observed n value can be correlated to the quantities in the interfacial layer model by Eqs. (5) and (6),

$$(q/nkT)=\gamma[1-\gamma(B/C)]/[1-(B/C)]. \tag{7}$$

Since γ defined by Eq. (2) involves D_s, Eq. (7) is solved to give

$$D_s=(\epsilon_i/\delta q^2)[1-(B/C)](n-1). \tag{8}$$

When the voltage dependence of (B/C) is neglected in Eq. (8), D_s is proportional to $(n-1)$. Exact values of the quantities, ϵ_i, δ, and (B/C) are unknown. As a rough estimate, we assume $\epsilon_i=4\epsilon_0$, ϵ_0 being the dielectric constant of vacuum, $\delta=20$ Å, and $B=C/2$. Although it is difficult to measure thickness δ exactly for GaAs, the oxide thickness δ of the Si MOS tunnel diode has been reported to be 20 Å.[6] The reason that $B=C/2$ is adopted is because $C=R+B$ and $R\cong B$ which is a condition where such an anomaly can be observed. The maximum observed value of n is about 3, then the maximum D_s becomes 1.1×10^{13} $(\mathrm{cm}^2\ \mathrm{eV})^{-1}$ by Eq. (8). Using these values, γ is obtained to be 0.5 from Eq. (2). In the next approximation, (B/C) decreases with increasing applied voltage. Hence, D_s increases with V in addition to the variation of $(n-1)$.

In order to represent the energy level of the interface states, its energy difference from the bottom of the conduction band E_c is used and is

$$E_c-E=q\phi_B-E_{Fi}=q[\phi_B-(\gamma/1-\gamma)(V+\Delta V_D)] \tag{9}$$

from Eq. (1). The value of $(V+\Delta V_D)$ in Eq. (9) can be obtained from experimental I-V data. Figure 3 illustrates the observed I-V curve and two ideal $n=1$ slopes, one of

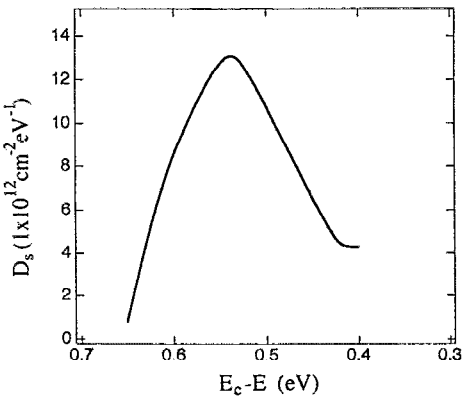

FIG. 4. Density of interface states D_s vs energy level E_c-E in sample B Schottky barrier.

which passes through the experimental curve at a low applied bias and the other passes through the experimental curve at an applied bias V. According to Eq. (3), ΔV_D is equal to the negative value of the applied voltage to an ideal Schottky barrier in which $\Delta\phi_B$ is equal to zero. Thus, $(V+\Delta V_D)$ is obtained as the separation of the two $n=1$ slopes.

Using the γ value estimated above, $\gamma/(1-\gamma)$ in Eq. (9) becomes unity. From the experimental n values shown in Fig. 1 and assuming (B/C) is 0.5, the distribution of D_s is obtained as shown in Fig. 4. The peak is at $E_c-E=0.54$ eV in good agreement with the values reported by Spicer *et al.*[5] from a photoemission experiment.

The above γ is very large and D_s is very small in comparison with $\gamma=0.07$ and $D_s=1.3\times10^{14}$ (cm^2 eV)$^{-1}$, respectively, hitherto accepted for the weak dependence of ϕ_B on the metal work functions.[1] In the surface Fermi level pinning where the interfacial layer model is applicable, the position of the neutral level ϕ_0 in the interface states is considered to be about 1/3 of the energy gap E_g from the top of the valence band E_v for most of the semiconductors. For GaAs, $E_g-q\phi_0$ was reported to be about 0.9 eV.[1] In our sample B, ϕ_B^0 was 0.66 V. Hence, an average D_s value in the energy range between $E_v+q\phi_0$ and E_F under zero bias plays a role in the surface Fermi level pinning. When the interface state density is analyzed as a function of its energy level, it is reasonable that the D_s value obtained here under forward bias for the interface states above E_{Fm} is different from that obtained for the surface Fermi level pinning. This consideration is consistent with the two peak positions of the interface states but is inconsistent with their relative magnitude given by the photoemission experiment.[5]

The reason the appreciable nonideal I-V characteristics were observed in the Schottky barrier of sample B but not in sample A is considered as follows; according to Eq. (8), the thickness δ of the interfacial layer was adequate in sample B to induce a remarkable potential difference in it and also to give a suitable ratio of (B/C). The present result rather implies that when a nonideal I-V characteristic of a Schottky barrier is observed having a maximum n-value in an intermediate range of applied voltage, it probably indicates a presence of a peak in the interface state density.

As a conclusion, the density distribution of interface states in a GaAs Schottky barrier was obtained for the first time from the nonideal I-V characteristics by the interfacial layer model. The result is that the energy position of the distribution peak and the absolute magnitude of the density are in agreement with those hitherto accepted values, when the energy distribution of the interface states and their role in the surface Fermi level pinning are considered.

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