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Theory of Non-Ideal I-V Characteristics of Schottky Barriers and Its Application to a-Si: H Schottky Barriers

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A new theory is developed for non-ideal I-V characteristics of Schottky barriers based on a model that electron population in the interface states is changed with applied voltage accompanying a change of the barrier height. This theory explains quantitatively experimental results of a-Si:H Schottky barriers and discloses interesting behavior of the Fermi level of the interface states as well as electronic transitions to and from the interface states.

1. INTRODUCTION

Schottky barrier diode is one of the most simple and basic semiconductor devices. However, its I-V characteritics cannot usually be explained by the theory of ordinary metal-semiconductor contact. The purpose of this study is to acquire knowledge of fundamental properties of Schottky barriers by investigating their non-ideal I-V characteristics.

Under conditions of Schottky barrier formation, the semiconductor surface is considered to be covered ordinarily with a thin layer of native oxide. The interfacial layer model[1)] of Schottky barrier successfully explains the dependence of the barrier height on the metal work functions. This explanation is based on the thermal equilibrium conditions at zero applied bias. When a bias voltage is applied, the Fermi level of the interface states E_{Fi} should be between the Fermi level of the metal E_{Fm} and that of the semiconductor bulk E_{Fs}. Depending on the position of E_{Fi}, the space charge at the interface and also the barrier height is considered to be varied.

In ordinary theories, the interfacial layer has been assumed to be thin enough for electrons to tunnel through with transmission coefficient T_T near unity. However, T_T is estimated to be very small[2)] for even thin layers of several atomic layer thick. Therefore, the carrier flow through the interfacial layer is considered to be a bottleneck and the I-V characteristics should be obtained from the flow of carriers through the interface.

A new theory of non-ideal Schottky barrier is developed from these viewpoints and is applied to a-Si:H Schottky barrier. Since undoped a-Si:H is a low-mobility semiconductor exhibiting large departure from the ideal Schottky characteristics, it is an appropriate material for investigating validity of the present theory.

This paper is a brief report and the detail is to be published elsewhere.[3)]

2. THEORY OF NON-IDEAL CHARACTERITICS

2-A. Change of Barrier Height

The interfacial layer model[1)] considers that the semiconductor and the metal

are separated by a thin insulating layer of thickness δ and dielectric constant ε_i. The interface state density is D_s/eV cm^2. When a bias voltage V is applied, the interface states are considered to be occupied to the Fermi level $E_{Fi}=(D_{sb}/D_s)qV$ relative to E_{Fm}, which is taken as zero level of energy. The energy band diagram is illustrated in Fig. 1.

The change of the barrier height ϕ_B is given by analyzing the interfacial layer model[3]

$$\Delta\phi_B=\phi_B-\phi_B^o=(1-\gamma)(D_{sb}/D_s)V, \quad (1)$$

and the change of the diffusion potential V_D is[3]

$$\Delta V_D=\Delta\phi_B-V=\{(1-\gamma)(D_{sb}/D_s)-1\}V. \quad (2)$$

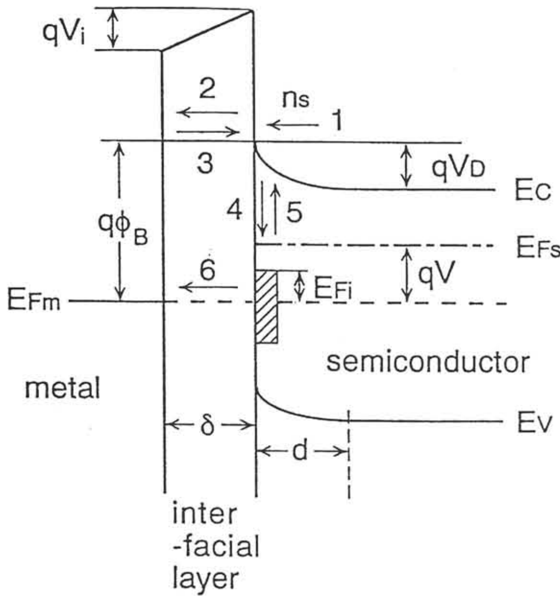

Fig. 1 Energy band diagram of Schottky barrier under forward bias V illustrating definitions of various quantities, electron flows and transitions. Shaded area indicates occupied interface states constituting space charge.

Here, $\gamma=1/\{1+(q\delta D_s)/\varepsilon_i\}$ is 0.25 from the dependence of ϕ_B^o on the metal work function.[4] The quantities involved in these equations are illustrated in Fig. 1 and the superscript denotes the value at zero bias.

In the above analysis, the space charge Q_D in the depletion region is neglected compared with the space charge Q_i in the interface states. It can be easily shown that Q_i is much larger than Q_D, because δ is much smaller than the depletion region width d while the potential drop V_i across the interfacial layer is of the same order of magnitude as V_D.

2-B. I-V Characteristics

Figure 1 also illustrates electron flows and transitions considered in the present model. The current is electron flow 1 being equal to the net tunneling current through the interfacial layer, flow 2 minus flow 3. The electron capture, transition 4, and the thermal release, transition 5, are approximately in a detailed balance under a steady state, since the rate of tunnel transition from the interface states to the metal, flow 6, is smaller than the rates of competing processes.

Under forward bias, the carrier density n_s at the interface is in thermal equilibrium with the bulk semiconductor because of small value of T_T as discussed later. By solving the current equations, the forward current for V>3kT/q is[3]

$$I=AT^2T_T\exp(-q\phi_B^o/kT)\exp(-q\Delta V_D/kT), \quad (3)$$

where A is the Richardson constant.

Under reverse bias, n_s decreases with increasing bias due to increased drift velocity into the bulk and the population in the interface states also decreases in thermal equilibrium with n_s. The reverse cur-

rent for $(D_{sb}/D_s)|V|>3kT/q$ is given by3)

$$I = A T^2 T_T \exp(-q\phi_B^0/kT)\exp(-q\Delta\phi_B/kT) \quad .(4)$$

Equations (3) and (4) express the same results as those of the thermionic emission theory except for the modifications introduced by the present theory; i.e., the factor T_T and the bias dependent exponential terms. Dependence of D_{sb}/D_s on V can be obtained by analyzing experimental results.

3. EXPERIMENTS AND ANALYSES

3-A. Sample Preparation

The samples used in this experiments are glass/ Cr/ undoped a-Si:H/ Ni-Cr structure. The a-Si:H film was deposited by PCVD. The Ni-Cr metal constituting the Schottky barrier was evaporated through a mask on freshly etched surface. The detail of sample preparation is described elsewhere.[3)]

3-B. Forward Characteristics

To represent the experimental results for small forward bias, the ideality factor n is used; i.e.,

$$I = I_0 \exp(-q\phi_B^0/kT)\exp(qV/nkT)\ , \qquad (5)$$

where I_0 is a constant. Equation (5) fits with theoretical Eqs. (2) and (3) by setting

$$D_{sb}/D_s = (n-1)/(1-\gamma)n\ . \qquad (6)$$

Figure 2 shows D_{sb}/D_s plotted against the forward current I, which is proportional to n_s. The curves are similar in shape and are displaced to higher currents at higher temperatures. For large currents, D_{sb}/D_s converges to unity. These behaviors of D_{sb}/D_s, i.e., the dependence of E_{Fi} on I, are understood by the relation[3)]

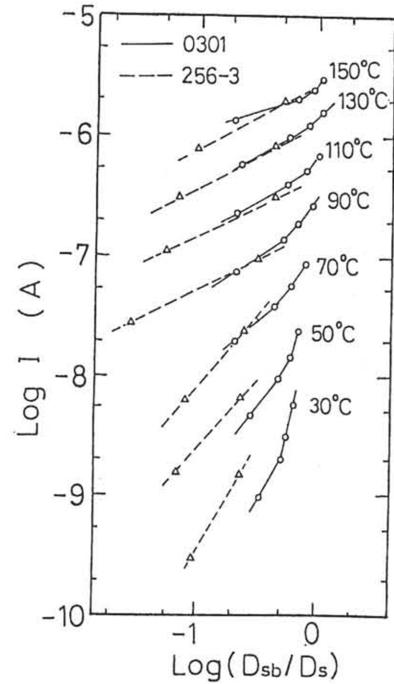

Fig. 2 D_{sb}/D_s vs forward current I for two samples at various temperatures. Sample numbers are 0301 and 256-3.

$$D_{sb}/D_s = C n_s / \{B^* + \nu\exp(-U/kT) + C n_s\}\ , \quad (7)$$

which is obtained by solving the rate equations of the electronic transitions to and from the interface states as illustrated in Fig. 1. Here, C is the capture coefficient, B^* is the tunneling probability to the metal, and $\nu\exp(-U/kT)$ is the thermal release probability into the conduction band. The experimental results imply an existence of small but finite B^*.[3)]

3-C. Reverse Characteristics

In Fig. 3, D_{sb}/D_s obtained by analyzing experimental data[3)] is plotted against V. Here, D_{sb} represents density of holes in the interface states normally occupied under zero bias. Values of D_{sb}/D_s are slightly dependent on temperature, decrease with V in an approximate proportionality to $1/\sqrt{V}$ and

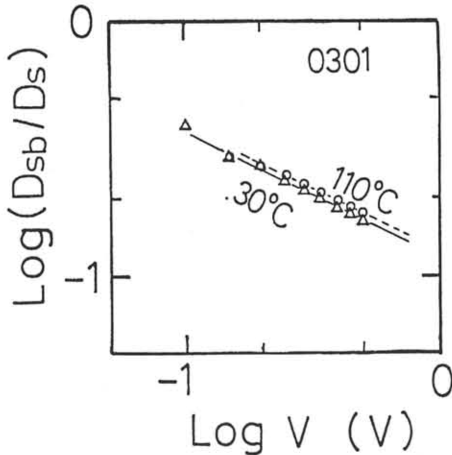

Fig. 3 D_{sb}/D_s vs reverse bias V at two temperatures.

extrapolate to unity roughly at V=kT/q. This result implys that the barrier height decreases proportionally to $\sqrt{V}$ with applied voltage.[3] This estimation of the decrease of the barrier height is in good agreement with the observed decrease of the activation energy of reverse current with increasing bias.[3]

4. DISCUSSION

For the I-V characteristics of undoped a-Si:H Schottky barriers, the departure from the ideal metal-semiconductor contact is quantitatively explained above by the present theory without taking other transport mechanisms and corrections into account. Consistency of the present theory is proved by the following relations among various quantities.

For a-Si:H, δ is considered to be about 10 A.[5] The magnitude of current in this theory is reduced by the factor T_T from the thermionic emission theory. Since ϕ_B=0.69 V for the present Schottky barrier, T_T is estimated[3] to be $5x10^{-5}$. This value is sufficient to assure the flatness of the quasi-Fermi level in the depletion region under forward bias. The introduction of T_T also resolves customary disagreement between ϕ_B values determined from the absolute value of I and from the temperature dependence of I.

The tunneling probability B^* from the interface states to the metal is compared with T_T.[3] The potential barrier for the former is larger than that for the latter by the barrier height ϕ_B. This is the reason why B^* is so small as considered in connection with Eq. (7).[3]

While the present theory is applied to a-Si:H Schottky barriers in this paper, it is expected to be also applicable to Schottky barriers of other semiconductors. Results of investigation of crystalline Si Schottky barriers with different surface treatments will be reported shortly.

5. CONCLUSION

The present theory and experiments clarify the mechanism of interface states making up the non-ideal I-V characteristics. They also form a new basis for future studies of Schottky barriers in connection with the interface states.

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