VOLUME 57, NUMBER 8 PHYSICAL REVIEW LETTERS 25 AUGUST 1986

Interface-State Measurements at Schottky Contacts: A New Admittance Technique

J. Werner[(a)]
IBM T.J. Watson Research Center, Yorktown Heights, New York 10598

and

K. Ploog and H. J. Queisser
Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 3 March 1986)

We present a new characterization method for traps at the interfacial layer of Schottky contacts. This method is based on ac-admittance measurements and a new trap transistor model which quantitatively explains the measured ac behavior as well as the dc characteristics. In particular we propose the ac current across the interface to consist of capacitive as well as of conductive parts. We apply the analysis to Au/GaAs Schottky contacts and find a weak energy dependence for the density of interface states in the band gap of GaAs.

PACS numbers: 71.20.+c, 73.30.+y

The simplest semiconductor device, the metal-semiconductor contact, is still inadequately understood. For an ideal junction a Schottky barrier $\Sigma_{\mathrm{id}} = \Phi_m - \chi$ is expected[1] between the two materials, where Φ_m is the metal's work function and χ the semiconductor's electroaffinity. Most Schottky contacts do not show this simple behavior and for GaAs interface dislocations have been proposed[2] to cause the deviation. The current controversy[3,4] about $\mathrm{NiSi_2}$-Si contacts might also be explained by interface defects. Interface states are therefore crucial, and appropriate experimental techniques for their characterization are urgently required.

Low-frequency capacitance was used to characterize interface states at Schottky contacts.[5] However, some doubts were raised earlier upon the consistency of the results.[6] The interpretation of such measurements usually refers to a classic admittance model[7] for metal-oxide-semiconductor (MOS) interfaces that describes trapping at the oxide/semiconductor interface. Carrier trapping by interface states is measurable and detectable as an induced displacement current in the oxide. The equivalent circuit[7] describes this by an interface-state conductance G_{ss} and a capacitance C_{ss} that are in parallel to the geometrical capacitance of the semiconductor's depletion region C_{sc} and in series to the oxide capactiance C_{int}. This model was recently[8] applied to interpret the low-frequency capacitance of *epitaxial* Schottky contacts *without* oxide or interfacial layer, by omission of the oxide capacitance C_{int} from the equivalent circuit. We feel that the effect of interface states at intimate Schottky contacts is more subtle and cannot simply be accounted for by omission of the oxide capacitance from the MOS circuit.

On the other hand, for Schottky contacts *with* an interfacial layer an application of the classic MOS model[7] seems to be justified. But even for this case the most striking difference between a MOS interface and a Schottky contact, namely the current *across* the interface and its influence on admittance, was not so far considered.

This Letter proposes a new interpretation for the ac properties of Schottky contacts with interfacial layers. We present a new meaurement technique for interface traps. Their energy distribution is derived from the frequency-dependent ac admittance of the current *across* the interface. We reveal a basic process that causes the observed frequency dependence and analyze our measurements within a transistorlike model. This model overcomes the inconsistencies[6] of other methods[5,8] and, moreover, it reproduces the classic dc model[9] for Schottky barriers as a special case for frequency $\omega = 0$.

Our analysis is here illustrated by measurements taken from Au/GaAs Schottky contacts because compound semiconductor Schottky contacts are characterized by pronounced interfacial layers.[10] We explain the deviation from the ideal behavior, $\Sigma_{\mathrm{id}} = \Phi_m - \chi$, by an interfacial dipole Δ between the metal and the semiconductor as shown in Fig. 1. Interface states at this dipole are capable of capturing free carriers from the semiconductor, becoming electrically charged, and thereby creating a barrier $\Sigma = \Phi_m - \chi - \Delta$.

The samples discussed consist of a 3.5-μm-thick, n-type GaAs layer, Si doped to $N_D = 2\times 10^{16}$ cm^{-3}, that is grown by molecular-beam epitaxy on GaAs substrates. After growth the samples are exposed to air and then Schottky contacts are formed by evaporation of 200-nm Au. This process produces the desired interfacial oxide as confirmed by the so-called ideality[9] $n = 1.35$ up to 0.5 V, $n = 6.2$ at 0.8 V, and a zero-bias barrier $\Sigma_0 = 0.92$ eV that we find from the dc characteristics. The measured capacitance yields a thickness of $\epsilon_r \times (36\ \text{Å})$ for the layer, where ϵ_r is its relative (static) dielectric constant.

Our analysis is based on the evaluation of the complex ac admittance $Y \equiv G + i\omega C$ with conductance G and capacitance C. Figure 2 shows the frequency-

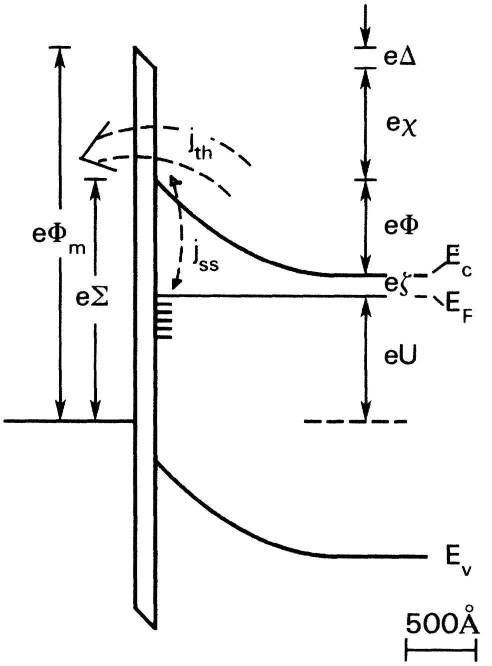

FIG. 1. Band diagram of a Schottky contact with an interfacial layer. Interface states are occupied up to the quasi-Fermi level E_F of free electrons at the interface. The current j_{th} emitted across the interface depends on band bending $e\Phi$ which in turn is controlled by the trapping current j_{ss}. This causes a transistorlike action of j_{ss} on j_{th}. The finite duration of the capture process results in a phase shift of the band-bending change $\delta\Phi$ with respect to an applied ac voltage δU. Frequency-dependent conductive (Fig. 2) *and* capacitive parts of j_{th} flow then across the interface.

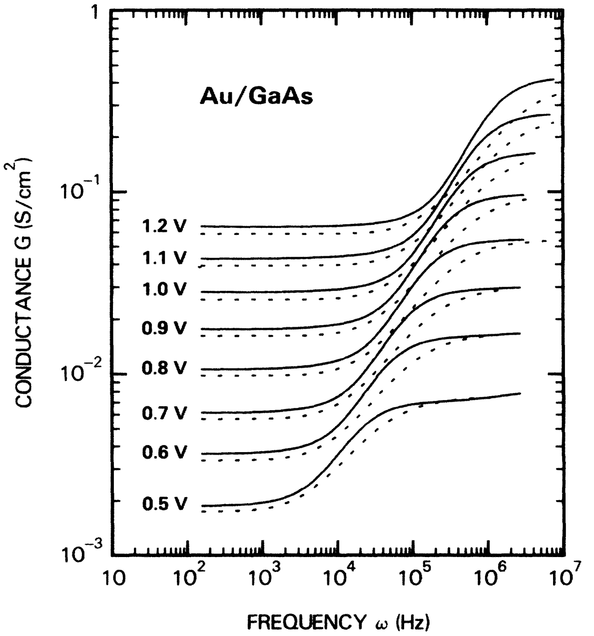

FIG. 2. Measured conductance G (solid curves) for different forward bias voltages U_{dc}. The frequency dependence is caused by a modulation of the current j_{th} across the interface (Fig. 1). From these curves information about the interface states is obtained by an analysis as shown in Fig. 3. Different bias voltages correspond to different energies of the Fermi level at the interface. Dotted curves originate from Eq. (8), after the determination of N_{ss}, σ from the maximum in Fig. 3.

dependent G of a contact measured with a Hewlett-Packard model 4192A *LCR* meter at 300 K. The low-frequency value, G_{dc}, agrees with the derivative of the dc current/voltage curve. The parallel capacitance C (not shown) is simultaneously measured.

We propose that the main part of the measured admittance of a Schottky contact with interface states is caused by the current j_{th} that flows at voltage U because of thermionic emission and subsequent tunneling *across* the interfacial layer of Fig. 1:

$$j_{th}=\Theta A^x T^2 \exp(-\Sigma/kT)\{\exp(eU/kT)-1\}. \quad (1)$$

Here A^x is an effective Richardson constant, kT/e is the thermal voltage, and Θ represents a tunneling factor.[9] The barrier Σ is related to the band bending $e\Phi$ and the bulk Fermi level $e\zeta$ by $e\Sigma=e\Phi+e\zeta+eU$. With $\rho=\Theta A^x T^2\exp(-e\zeta/kT)$ we get for $U_{dc} >> kT/e$

$$j_{th}=\rho\exp(-e\Phi/kT). \quad (2)$$

The band bending Φ and thus the Schottky barrier Σ vary with voltage (and time), according to the respective voltage drops over interfacial layer and space-charge region. The whole band diagram in Fig. 1, i.e., the field strengths, is only restricted by Maxwell's equations and overall charge neutrality. The actual areal[11] trapped interface charge, Q_{ss}, is to be balanced by the charge within the semiconductor's space-charge region, Q_{sc}, and the charge on the metallic side of the interface, Q_m:

$$eQ_{ss}=-(eQ_m+eQ_{sc})=\epsilon_{int}E_{int}-\epsilon_{sc}E_{sc}. \quad (3)$$

The second part of Eq. (3) follows from Gauss's law and ϵ_{int}, ϵ_{sc} and E_{int}, E_{sc} represent the dielectric constants and the (maximum) field within interfacial layer and space-charge region, respectively.

We find the ac current across the interface from a small-signal analysis of Eq. (2): The application of an ac voltage depending on time t as $\delta U(t)=\delta\tilde{U}\times\exp(i\omega t)$ with $\delta\tilde{U} << kT/e$ in addition to a dc bias U_{dc} results in a time-periodic change of the band bending $\Phi(t)=\Phi_{dc}-\delta\Phi(t)$. With $\delta\Phi << kT/e$ one gets a current

$$j_{th}(t)=j_{dc}^{th}[1+e\delta\Phi(t)/kT]=j_{dc}^{th}+\delta j_{ac}(t), \quad (4)$$

where

$$\delta j_{ac}(t)=j_{dc}^{th}e\delta\Phi(t)/kT. \quad (5)$$

Here $j_{dc}^{th} = \rho \exp(-e\Phi_{dc}/kT)$ is used and Eq. (5) describes the ac current δj_{ac} across the interfacial layer. Note that δj_{ac} is in phase with and directly proportional to $\delta\Phi$ and *not* to δU. The quantity $\delta\Phi$ is neither equal to δU (a part of the voltage drops at the interfacial layer) *nor even in phase* with δU. The whole band diagram in Fig. 1, including the magnitude and the phase of $\delta\phi$, is *not* fixed by the applied voltage δU but exclusively by overall charge neutrality, Eq. (3). This key consideration distinguishes our model from previous work[5,8] and avoids inconsistencies[6] due to a violation of charge neutrality, Eq. (3). Charge neutrality generally must result in an out-of-phase component of $\delta\Phi$. Only this guarantees for MOS interfaces the measurability of interface states with the help of displacement currents. For Schottky contacts, according to Eq. (5), this results, in addition, in *capacitive currents.*

The dependence of $\delta\Phi$ on δU is found from an analysis of the current j_{ss} that is exchanged between the conduction band and the interface traps as a result of the capture and emission of electrons. The current j_{ss} is measurable as a small displacement current in the interfacial layer. It is identical to the time derivative of the trapped interface charge Q_{ss}, and this current j_{ss} controls the actual band bending $\delta\Phi$ and therefore the current δj_{ac} in Eq. (5)! Thus the current j_{ss} acts on the thermionic current j_{th} in a similar way as the base current in a transistor acts on the collector current (trap transistor action).

We assume a flat quasi-Fermi level for electrons, neglect the recombination of electrons with holes, and express j_{ss} in terms of a conductance, G_{ss}, and a capacitance, C_{ss}[7]:

$$j_{ss}(t) = \frac{dQ_{ss}(t)}{dt} = (G_{ss} + i\omega C_{ss})\delta\Phi(t). \tag{6}$$

A small-signal analysis of Eq. (3) with $C_\Sigma = C_{sc} + C_{int}$ yields

$$\begin{aligned} j_{ss}(t) &= e\, dQ_{ss}(t)/dt \\ &= i\omega C_{int}\delta U(t) - i\omega C_\Sigma \delta\Phi(t). \end{aligned} \tag{7}$$

We solve Eqs. (6) and (7) for $\delta\phi$ and get, with $C_{hf}^{-1} = C_{int}^{-1} + C_{sc}^{-1}$, for the measured admittance $Y = G + i\omega C \equiv \delta j_{ac}/\delta U + i\omega C_{hf}$

$$G = \frac{j_{dc}^{th}}{kT/e} \frac{C_{int}(C_\Sigma + C_{ss})}{(C_\Sigma + C_{ss})^2 + (G_{ss}/\omega)^2}, \tag{8}$$

$$C = \frac{j_{dc}^{th}}{kT/e} \frac{C_{int} G_{ss}/\omega^2}{(C_\Sigma + C_{ss})^2 + (G_{ss}/\omega)^2} + C_{hf}. \tag{9}$$

In the derivation of Eqs. (8) and (9) we have neglected the *direct* influence of the current j_{ss} on admittance Y. An exact analysis[12] shows that this effect can usually be neglected for current-carrying interfaces.

The measured G and C in Eqs. (8) and (9) depend on frequency because G_{ss} and C_{ss} depend on frequency and the latter two quantities contain information about the interface states. We extract G_{ss}, C_{ss} therefore from the measured G, C, and then we subject them to an analysis. They are related to the density of interface states, N_{ss}, and the capture cross section, σ, by

$$G_{ss} = e^2 N_{ss}(2\tau)^{-1} \ln(1 + \omega^2\tau^2)$$

and

$$C_{ss} = e^2 N_{ss}(\omega\tau)^{-1} \arctan(\omega\tau),$$

where $\tau^{-1} = v\sigma N_D \exp(-e\Phi_{dc}/kT)$, and v is the thermal velocity. The quantities G_{ss} and C_{ss} contain the same information about the interface states since they fulfill the Kramers-Kronig relations. The latter applies because we use a causal and linear small-signal model. It is therefore sufficient to extract and to analyze G_{ss}. Solving of Eqs. (8) and (9) for G_{ss} yields

$$G_{ss} = \frac{j_{dc}^{th}}{kT/e} \frac{\omega^2 C_{int}(C - C_{hf})}{G^2 + \omega^2 (C - C_{hf})^2}. \tag{10}$$

The value for C_{int} is obtained from the high-frequency values of G and C and then the evaluation is carried out as shown in Fig. 3. Results for N_{ss} are shown in

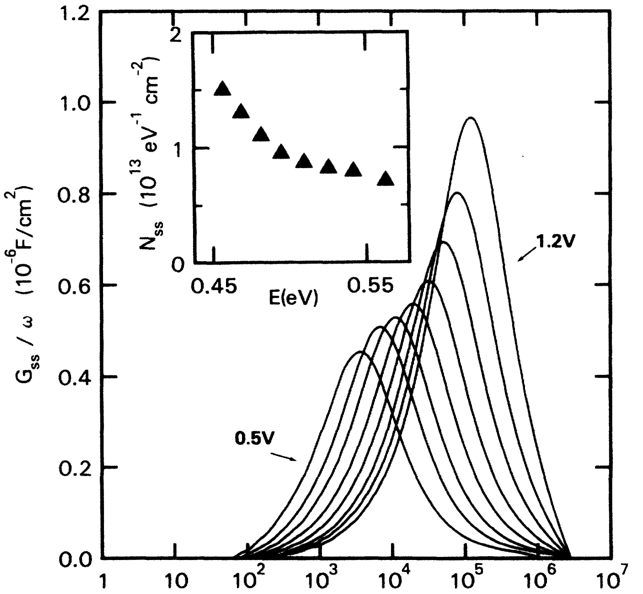

FIG. 3. The quantity G_{ss}/ω of the current j_{ss} as calculated from the measured G, C with the help of Eq. (10) for the voltages of Fig. 2. The curves go through maxima at $\omega\tau = 1.98$ with values of $0.4e^2N_{ss}$. The ordinates and frequencies of the maxima yield therefore density of interface states, N_{ss}, and capture cross section, σ. The inset shows results obtained. The energy E in the band gap is measured from the band edge E_c at the interface (Fig. 1).

the inset. For the capture cross section we find $\sigma = 2\times 10^{-13}$ cm^2.

The present model describes the whole frequency dependence of the admittance. It is interesting, therefore, to consider the special cases of low and high frequencies. At high frequencies the first term in Eq. (9) vanishes and there remains only the term C_{hf} due to the geometric series capacitances of interfacial layer and space-charge region. The connection to the dc conductance G_{dc}, i.e., to the slope of the current-voltage curve, is, on the other hand, found from Eq. (8) for $\omega = 0$. We then get the ideality n of the current-voltage curve as

$$n \equiv e j_{\text{dc}}^{\text{th}} / kT G_{\text{dc}} = 1 + C_{\text{int}}^{-1}\,(C_{\text{sc}} + e^2 N_{\text{ss}}).$$

This equation has the same meaning as Eq. (18) in the paper of Card and Rhoderick[9] about the dc properties of Schottky contacts. The values for N_{ss} that we deduce from the behavior G_{ss}/ω in Fig. 3 agree with those from the ideality n of the current-voltage curve. Hence, our general admittance model reproduces the classic dc theory[9] as a special case for $\omega = 0$.

On the other hand, our model differs considerably from the usual interpretation[5,8] that (even for Schottky contacts without interfacial layer) assumes the frequency-dependent admittance somehow to be *directly* influenced by trapping at the interface. In previous work[5] the density of interface states was inferred from the low-frequency capacitance C_{dc}, by use of $C_{\text{dc}} = e^2 N_{\text{ss}}$. This is impossible within our model which proposes the main part of the admittance to be caused by the *indirect* action of the capture/emission current j_{ss} upon the current j_{th} *across* the interface via the control of interface charge and bond bending. Within our amplification model the low-frequency value of the capacitance, C_{dc}, is obtained from Eq. (9) for $\omega = 0$:

$$C_{\text{dc}} = \frac{j_{\text{dc}}}{2kT/e}\,\frac{C_{\text{int}} e^2 N_{\text{ss}} \tau}{(C_\Sigma + e^2 N_{\text{ss}})^2} + C_{\text{hf}}. \tag{11}$$

A measurement[5,8] of C_{dc} is therefore *not* sufficient for deducing N_{ss}. From a high capacitive current at low frequencies[8] one *cannot* infer a high value for the density of states, because τ has to be known first. The time constant in turn depends strongly on bias as shown in Fig. 3.

In conclusion, we propose a consistent transistorlike model for the characterization of interface traps at Schottky contacts. It considers the influence of the capture/emission current j_{ss} at the interface upon the current j_{th} across the interface via charge and barrier control. Our model permits the determination of the energy distribution as well as the capture cross section of interface states at Schottky contacts with an interfacial layer.

We acknowledge the support of P. S. Ho and thank J. L. Freeouf, A. B. Fowler, M. Liehr, M. Wittmer, and H. L. Evans for discussions.

---

[a] On leave from Max-Planck-Institut für Festkörperforschung, Stuttgart, West Germany.

[1] W. Schottky, Z. Phys. **118**, 539 (1942).

[2] J. M. Woodall, G. D. Pettit, T. N. Jackson, C. Lanza, K. L. Kavanagh, and J. W. Mayer, Phys. Rev. Lett. **51**, 1783 (1983).

[3] R. T. Tung, Phys. Rev. Lett. **52**, 461 (1984).

[4] M. Liehr, P. E. Schmid, F. K. LeGoues, and P. S. Ho, Phys. Rev. Lett. **54**, 2139 (1985).

[5] C. Barret and A. Vapaille, J. Appl. Phys. **50**, 4217 (1979).

[6] J. L. Freeouf, Appl. Phys. Lett. **41**, 285 (1982).

[7] E. H. Nicollian and A. Goetzberger, Bell. Syst. Tech. J. **46**, 1055 (1967).

[8] P. S. Ho, E. S. Yang, H. L. Evans, and X. Wu, Phys. Rev. Lett. **56**, 177 (1986).

[9] H. C. Card and E. H. Rhoderick, J. Phys. D **4**, 1589 (1971).

[10] L. J. Brillson, Surf. Sci. Rep. **2**, 123 (1982).

[11] Q_{ss}, Q_{sc}, and Q_m have the unit cm^{-2}.

[12] J. Werner, unpublished.