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CURRENT TRANSPORT AND ITS EFFECT ON THE DETERMINATION OF THE SCHOTTKY-BARRIER HEIGHT IN A TYPICAL SYSTEM: GOLD ON SILICON

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Abstract—The measurements of photovoltage, internal photoemission, current–voltage (I–V) and capacitance–voltage (C–V) have been performed for Au on n-Si (111) within a temperature range of 7 to 300 K. The values of Schottky-barrier height at room temperature obtained from these four measurements are in very good agreement, but conflicting results have been obtained at low temperatures. The measurements of both the internal photoemission and the C–V show a negative temperature dependence of the barrier height which is almost identical to that of the indirect energy band gap in silicon, but the barrier height obtained from the photovoltage measurements and the I–V measurements strongly decreases as temperature decreases. In this paper, the influence of the current transport on the determination of the Schottky-barrier height is discussed, and it is demonstrated that the conflicting results may be explained well in terms of the recombination current involved in the photovoltage measurements and the I–V measurements.

1. INTRODUCTION

Any theoretical model of the Schottky-barrier formation relies on reliable data on the Schottky-barrier height (SBH). However, a careful survey of the literature reveals that conflicting results exist in many experiments concerning the SBH [for example 1–14]. It can be seen from the literature that the SBH values obtained from the current–voltage (I–V) measurements, capacitance–voltage (C–V) measurements, and internal photoemission measurements are generally different; this holds for chemically clean surfaces as well as for UHV-cleaved surfaces. For its simplicity the I–V measurement is the most popular and common technique[15]. However, this technique is based on the assumption that the thermionic emission over the Schottky-barrier is the only current transport process at the metal/semiconductor interface. It has been observed that the I–V characteristics of certain Schottky diodes deviate from the thermionic-emission theory due to the contribution of other current transport processes, particularly the contribution of the recombination current of the carriers in the depletion region[14–16]. Therefore, a complete understanding of the current transport at the metal–semiconductor interface is fundamental for the reliable determination of the barrier height. Important information can be obtained from the temperature dependence of the electrical and photovoltaic characteristics of Schottky diodes. This allows us to identify the current transport processes involved using their particular temperature dependence. It is our attempt in this work to study the current transport and its influence on the determination of the Schottky-barrier height in the I–V and photovoltage measurements through the investigation of the temperature dependence.

In the present work, Au/n-Si (111) as a typical system has been studied. The measurements of I–V, C–V, internal photoemission, and photovoltage have been carried out at various temperatures. In this work, the SBH values have been obtained not only from the conventional measurements of I–V, C–V, and internal photoemission, but also from the measurement of the photovoltage. It will be shown that the SBH obtained from both the C–V and the internal photoemission measurements has a negative temperature dependence which is almost identical to that of the indirect energy band gap in silicon while the SBH from the I–V and the photovoltage measurements has a strong positive temperature dependence, and that this conflict is due to the neglect of the contribution of the recombination current involved in the I–V and the photovoltage measurements. It will be shown also that the contribution of the recombination current strongly depends on temperature and the sample's annealing experience.

2. EXPERIMENTAL

The substrates used in this study are n-type ($1 \times 10^{15}\,cm^{-3}$) silicon wafers of (111) orientation. The silicon wafers are cleaned with a standard chemical cleaning procedure which includes a final dip in diluted HF, as described by Taubenblatt *et al.*[18]. A low resistivity Ohmic back contact is made by using Au–Sb alloy. For the I–V and C–V measurements, 1000 Å of Au films are evaporated onto the Si wafers to form circular spots with 3 mm diameter.

For the photovoltage and the internal photoemission measurements, the thickness of the Au films used is 150 Å and the diameter of the circular spots is in the range of 4–6 mm.

In the I–V measurements, the voltage applied to the Schottky diodes is from a programmable voltage generator (HP3245A) and the current through the diodes is measured with a digital pico-ammeter (Keithley 485). In the C–V measurements, a direct capacitance bridge (Model 75B-S8, Booton Electronics) is used. Both the I–V measurements and the C–V measurements were carried out inside a well-regulated liquid nitrogen (Oxford Instrument) cryostat.

In the photovoltage and the internal photoemission measurements, a monochromatic beam is provided by a grating monochromator with a grating of 300 lines/mm and equipped with a Si long-pass i.r. filter. The beam is well focused through two CaF_2 lenses onto the samples. The incident photon flux at each energy is determined by a pyroelectric photodetector. All the measurements are performed in darkness, but the dark signal is also subtracted. In the photovoltage measurements, the incident photon energy is fixed at 1.20 eV. The "open circuit" photovoltage is measured with a Keithley electrometer with $10^{14}\,\Omega$ input impedance and the "short circuit" photocurrent is measured with a pico-ammeter as in the I–V measurements. In the internal photoemission measurements, the incident beam is modulated by a chopper, and the modulated photocurrent on a loaded resistor is detected by a lock-in amplifier (EG&G 9503-SC). Both the photovoltage and the internal photoemission measurements are carried out with the HS-4 HELIPLEX® refrigeration system in which the temperature of the samples is well controlled in the range of 4–300 K.

3. RESULTS AND DISCUSSIONS

3.1. The I–V measurements

The I–V characteristics of a Schottky diode is normally described with the well-known thermionic-emission equation[15]:

$$J = J_0 \exp(qV/nkT)[1 - \exp(-qV/kT)], \quad (1)$$

where $J_0 = A^*T^2 \exp(-q\Phi_b/kT)$, A^* is the Richardson constant and n is the ideality factor which describes the deviation of practical diodes from the pure thermionic-emission model characterized by $n = 1$.

Based on (1), the SBH values (Φ_b) for the Au/n-Si samples are determined by extrapolating the forward I–V curves to zero applied voltage. The extrapolation is made by a linear fit over 3 orders of magnitude or greater of the current. The slope of the linear portion yields the value of the ideality factor n. The SBH values evaluated with $A^* = 1.12 \times 10^6\,\mathrm{A\,m^{-2}\,K^{-2}}$ are shown in Fig. 1 by the empty triangles as a function of temperature, and the temperature dependence of

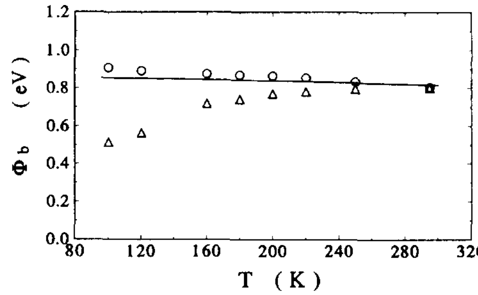

Fig. 1. Temperature dependence of the barrier height values for Au/n-Si sample and the variation of the indirect band gap in silicon (—) with temperature. The open circles: the SBH values obtained from the C–V measurements. The open triangles: the SBH values obtained from the I–V measurements.

the n factor is plotted in Fig. 2. At room temperatures, the SBH obtained is 0.80 eV which is in very good agrement with the values obtained from the C–V, the photovoltage and the internal photoemission measurements. The diodes display a near-unity ideality factor ($n = 1.1$). However, as the temperature decreases, the SBH value obtained decreases and the n factor increases. At 100 K, the SBH and the n factor reach a value of 0.51 and 1.97 respectively. The strong increase of the n factor at low temperatures, together with the decrease of the Schottky-barrier height conflict with the results from the C–V and the internal photoemission measurements discussed below. This indicates that the Schottky diodes have deviated from the thermionic-emission theory and that other current transport processes may play a significant role at low temperatures. As discussed in Section 3.4, other current transport processes, i.e. the tunneling current through the barrier, the recombination current in the depletion region, and the leakage current, may have their contributions to the total current transport at the metal/semiconductor interface[14,19,20].

In order to justify the influence of the tunneling current, we make a quantitative estimate of the relative importance of the thermionic-emission current and the tunneling current for the material used in the present study. The relevant parameter in the

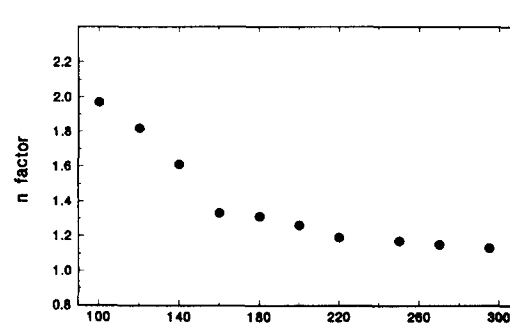

Fig. 2. Temperature dependence of the ideality factor for Au/n-Si sample.

determination of the tunneling probability out of the semiconductor bulk is the quantity E_{00} which, for electrons at the edge of the depletion region is given by [15]:

$$E_{00} = 18.5 \times 10^{-15} (N_d/m_r \epsilon_r)^{0.5}, \tag{2}$$

where m_r is the electron effective mass, ϵ_r is the relative dielectric constant of semiconductors, and N_d is the donor concentration. As an approximate guide, comparing with the thermionic-emission current, the tunneling current becomes important when $E_{00} > kT$. For the n-Si wafers used in this study, $N_d = 1 \times 10^{15}\,\text{cm}^{-3}$ which leads to values of $E_{00}/kT = 0.01$ at 300 K and $E_{00}/kT = 0.03$ at 100 K. Therefore, the influence of the tunneling current is insignificant in the I–V measurements of these Schottky diodes.

The leakage current may have some influence on the I–V characteristics of the Schottky diodes. However, after careful checks, this has been ruled out in our experiments. Details will be discussed in Section 3.4.

The recombination current in the depletion region has been reported to be an important factor responsible for the deviation of the I–V characteristics from the behaviour described by the thermionic-emission theory[16,17]. The recombination of the electrons and holes normally takes place via localized centers with energies which are near the center of the band gap (a typical example of such an efficient recombination centre is gold in silicon[21,22]), and it is expected in Schottky diodes with high barriers, at low temperature, and low forward-bias voltage[10,15]. Obviously, the contribution of the recombination current to the total current transport should have its influence on the determination of the Schottky barrier height in the I–V measurements. Here we give an estimate on such an influence. It is assumed that, the total current J consists of the thermionic-emission J_{th} and the recombination current J_{rec}, i.e. $J = J_{th} + J_{rec}$, and the thermionic-emission current obeys the pure thermionic-emission theory ($n = 1$). If the recombination current is ignored, a SBH value Φ_b' will be obtained based on:

$$J = A^*T^2 \exp(-q\Phi_b'/kT)[\exp(qV/kT) - 1]. \tag{3}$$

If the recombination current is included, then a different SBH value Φ_b will be obtained based on:

$$J = A^*T^2 \exp(-q\Phi_b/kT)[\exp(qV/kT) - 1] + J_{rec}. \tag{4}$$

Under the above assumptions, the value Φ_b should represent the "true" barrier height. From (3) and (4), the difference between the two SBH values can be expressed as:

$$q\Phi_b - q\Phi_b' = -kT \ln(1 - J_{rec}/J). \tag{5}$$

As a rough estimate, if the recombination current contributes 30% to the total current at room temperatures, $q\Phi_b'$ will be less than $q\Phi_b$ by 10 meV; if the recombination current contributes 99.9% to the total current (i.e. the recombination current is larger than the thermionic-emission current by 3 orders of magnitude) at 200 K, $q\Phi_b'$ will be less than $q\Phi_b$ by 0.12 eV. Obviously, neglecting the contribution of the recombination current will lead to a lower barrier height being obtained. It can be expected that the SBH values determined from the thermionic-emission theory will decrease as the temperature decreases since the recombination current will be more significant at lower temperatures. This is the case that we observe in the I–V measurements which shows a positive temperature dependence of the SBH obtained as shown in Fig. 1.

3.2. The C–V measurements

Based on the dependence of the barrier capacitance C on the applied bias voltage V, the diffusion potential V_d of the barrier can be obtained from a plot $1/C^2$ vs V, and the Schottky-barrier height is determined from [11,15,21]:

$$q\Phi_b = qV_d + qV_n \tag{6}$$

where qV_n is the energy difference between the bulk CBM and the bulk Fermi level, which is a function of temperature[21]. A very good linear dependence of $1/C^2$ on the reverse bias voltage is obtained for the Au/n-Si diodes in the voltage range of 0–1.5 V. The slope of the $1/C^2$ vs V curves is almost unchanged in the measured temperature range and yields the donor concentration N_d as $1 \times 10^{15}\,\text{cm}^{-3}$ agreeing very well with the nominal value. The barrier height values derived from the C–V measurements are shown in Fig. 1 by the open circles. It can be seen from Fig. 1 that, although the SBH value obtained at room temperature is in very good agreement with that from the I–V measurements, the temperature dependence of the SBH obtained at low temperatures conflicts with the results from the I–V measurements. The SBH from the C–V measurements increases as the temperature decreases with a coefficient almost identical to that of the indirect band gap in silicon as shown in Fig. 1, and this positive temperature dependence of SBH is consistent with the results from the internal photoemission measurements. This temperature dependence of SBH in Au/n-Si Schottky diodes obtained from our C–V and internal photoemission measurements coincides with that reported by Crowell *et al.*[8]. They point out that such a temperature dependence of SBH implies the Fermi level being pinned in relation to the VBM at the Au–Si interface. For other metals such as tungsten on silicon, it is also reported that the Fermi level at the interface is pinned relative to the VBM[27]. Up to now, several models have been proposed to explain the Fermi level pinning[13,27]. Particularly, the Fermi level pinning may be due to defects, as shown by Van Meirhaeghe *et al.*[28]. Although the issue of Fermi level pinning is of great interest to us, it is not in the scope of the present paper.

3.3. The internal photoemission measurements

Based on the Fowler theory[24], the square root of photocurrent normalized by unit incident photon vs photon energy gives a direct determination of the Schottky-barrier height by the extrapolation of the linear portion of the curves to zero photocurrent [25]. The square root of the photocurrent (in arbitrary units) in Au/n-Si diodes vs photon energy is shown in Fig. 3. The intersection of the extrapolation with the energy axis gives the SBH values at different temperatures, and this intersection simply moves towards higher energy as the temperature decreases indicating an increase of the SBH with decreasing temperature. The SBH obtained at 7 K is 0.84 eV which is 70 meV higher than that at 300 K. The variation of the SBH obtained from the internal photoemission measurements as a function of temperature is shown in Fig. 4 by the solid triangles. It is clearly evident from Fig. 4 that this variation of the SBH with temperature is identical to the temperature dependence of the indirect band gap in silicon. The internal photoemission measurements also show that, the annealing of samples does not change the temperature dependence of the SBH, nor does it change the barrier height significantly. The annealing at 100°C for 10 min and at 200°C for 30 min leads to only a very small shift of SBH with 10 meV and 15 meV, respectively. These results are conflicting with those from the photovoltage measurements, and the comparison of the results from these two kinds of measurements leads to an insight into the influence of the current transport on the determination of the Schottky barrier height, as discussed below.

3.4. The photovoltage measurements

Under light illumination with photon energy larger than the energy band gap in the semiconductor, photon absorption generates electron–hole pairs in the depletion region, these electron–hole pairs are separated by the built-in field of the Schottky-barrier and thus a photovoltage V across the depletion region

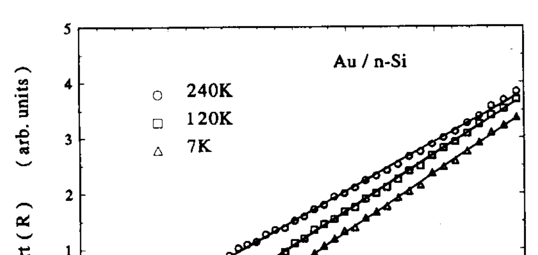

Fig. 3. Square root of the normalized photocurrent (in arbitrary units) in the Au/n-Si samples vs photon energy.

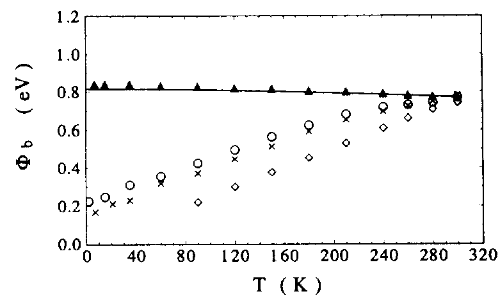

Fig. 4. Temperature dependence of the indirect band gap in silicon (—) and of the SBH values. The solid triangles: the SBH values (the unannealed sample) obtained from the internal photoemission measurements. The SBH values obtained from the photovoltage measurements are shown by the open circles (the unannealed sample) and × (the sample annealed at 100°C for 10 min) as well as the open diamonds (the sample annealed at 200°C for 30 min).

is produced. Meanwhile, the generation and the separation of the electron–hole pairs also produce a photocurrent J_{pc} in the depletion region. In equilibrium (steady state), the generated photocurrent is countered by a restoring current J which includes mainly the thermionic-emission current J_{th} over the barrier, the tunneling current J_{tu} through the barrier, the recombination current J_{rec} in the depletion region, and the leakage current J_{le}[14,19]:

$$J_{pc} = J = J_{th} + J_{tu} + J_{rec} + J_{le}. \quad (7)$$

In an early study[19], we have studied the leakage current effect on the photovoltage. In the present work, particular attention is paid to avoid the influence of the leakage current. The leakage resistance of our samples is estimated to be larger than $10^8\,\Omega$, and thus the leakage current should not have significant influence on the photovoltage[23]. In case of the diodes being shorted by an external circuit (i.e. the resistance of the external circuit is zero or much smaller than the internal resistance of the diodes), the "short circuit" current is equal to the photocurrent. Therefore, the photocurrent J_{pc} can be measured with a pico-ammeter with very low input impedance.

As the leakage current has no significant influence in the present measurements, it is eliminated from (7) in the following calculations. If the recombination current has no contribution to the total restoring current or in fact it is ignored by one, (7) becomes as:

$$J_{pc} = J = J_{tu} + J_{th}. \quad (8)$$

The contribution of the tunneling current and the thermionic-emission current is determined with the thermionic-field emission solution[15], and thus (8) is written as:

$$J_{pc} = J = J_s \exp(V/E_0)[1 - \exp(-qV/kT)]. \quad (9)$$

The mathematical expressions for E_0 and J_s can be found in Ref. [15]. Note that the saturation current J_s is a function of Schottky-barrier height Φ_b and (9) can be used in a general case (from low doping concentration to high doping concentration). But for the case of low doping concentration which applies to our samples with N_d of $1 \times 10^{15}\,\text{cm}^{-3}$, the tunneling effect is not important, and thus the tunneling current can be neglected. In this case, (8) can be written as:

$$J_{pc} = J = J_{th} = A^*T^2 \exp(-q\Phi_b/kT) \times [\exp(qV/kT) - 1]. \quad (10)$$

Using the experimental data of the photocurrent J_{pc} and the photovoltage V, the barrier height $q\Phi_b$ is computed with both (9) and (10). As expected for our samples, it is found that there is no significant difference between the $q\Phi_b$ computed with (9) and the $q\Phi_b$ computed with (10). The SBH value obtained as a function of temperature is shown in Fig. 4. For the unannealed samples, the SBH value obtained at room temperature is 0.77 eV which is equal to the value obtained from the internal photoemission measurements, but it decreases strongly as temperature decreases and it reaches a value of 0.23 eV at 7 K. As it can be seen in Fig. 4, low temperature ($\leqslant 200°$C) annealing greatly enhances such a decrease of the SBH values obtained at low temperatures although it has no significant influence on the SBH as obtained from the internal photoemission measurements. As pointed out below, this phenomenon relates to the influence of the recombination current involved in the photovoltage measurements.

Obviously, the temperature dependence of the SBH obtained from the photovoltage measurements is similar to that from the I–V measurements. In the theoretical treatments for both measurements, the recombination current is not included although it can cause a strong positive temperature dependence of the SBH obtained as discussed in Section 3.1. As a result, it is necessary to examine the variation of the contribution of the recombination current to the total current with temperature.

Using the SBH values obtained from the internal photoemission measurements which are performed with the photovoltage measurement in the same experimental arrangement, we are able to calculate the contribution of the thermionic-field-emission current (as discussed in Section 3.1, for our samples, there is no significant difference between the thermionic-field-emission current and the thermionic-emision current) involved in the photovoltage measurements. Since the leakage current has been ruled out in the measurements, and based on (7), the contribution of the recombination current to the total current is generally expressed as:

$$\frac{J_{rec}}{J} = \frac{J_{rec}}{J_{pc}} = 1 - \frac{J_{th} + J_{tu}}{J_{pc}}, \quad (11)$$

where in case of low doping concentration, J_{tu} can be neglected. The temperature dependence of the contribution of the recombination current is calculated using (11), and the result is shown in Fig. 5. As it can be seen in Fig. 5, for the unannealed sample, at room temperatures, the recombination current has no significant contribution to the total current (the thermionic-field emission current is larger than the recombination current by more than two orders of magnitude), indicating that the determination of SBH in the photovoltage measurements is almost unaffected by the recombination current. The coincidence of the SBH value obtained at room temperatures from the photovoltage measurements with that from the internal photoemission measurements strongly supports this argument. However, as shown in Fig. 5, the contribution of the recombination current increases rapidly as temperature decreases and becomes dominant at not too low temperatures. Such a rapid increase of the contribution of the recombination current at low temperatures has a serious influence on the determination of SBH in the photovoltage measurements and leads to a decrease of the SBH obtained as temperature decreases. In other words, at low temperatures the increase of the contribution of the recombination current shown in Fig. 5 is responsible for the decrease of the SBH obtained as shown in Fig. 4. The situation is similar to that in the I–V measurements as discussed in Section 3.1.

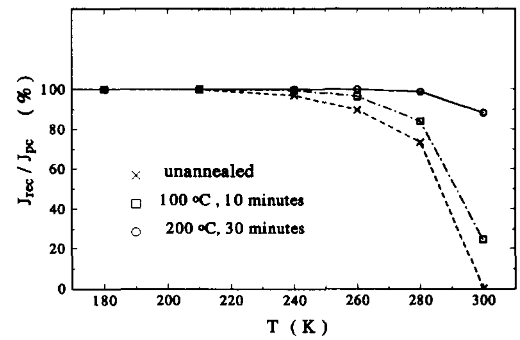

Fig. 5. Temperature dependence of the contribution of the recombination current to the total current for the samples which are respectively unannealed (×), annealed at 100°C for 10 min (□), and annealed at 200°C for 30 min (○).

As shown in Fig. 5, the low temperature annealing of the samples causes a large increase of the contribution of the recombination current. For example, at room temperatures, the recombination current in the unannealed samples almost has no contribution to the total current, but it contributes 87% to the total current in the samples which have been annealed at 200°C for 30 min. This indicates that the recombination of the carriers in the depletion region is enhanced by the annealing. As the contribution of the recombination current leads to a lower SBH, this enhancement of the recombination should be responsible for the stronger positive temperature dependence of the SBH obtained from the photovoltage measurements caused by annealing as mentioned above.

4. CONCLUSIONS

The measurements of photovoltage, internal photoemission, $I-V$, and $C-V$ have been performed for Au/n-Si in a wide range of temperatures. Both the $C-V$ measurements and the internal photoemission measurements, which are believed to yield more reliable SBH values in the present study as they are not affected by the current transport uncertainties, show a negative temperature dependence of the SBH which is identical to that of the indirect band gap in silicon. On the other hand, the SBH obtained from the photovoltage measurements and the $I-V$ measurements has a strong positive temperature dependence. It is demonstrated that, the determination of the SBH in the $I-V$ and the photovoltage measurements is seriously affected by the recombination current, and the contribution of the recombination current leads to a lower SBH value. Low temperature annealing of the samples increases the contribution of the recombination current and thus enhances the positive temperature dependence of the SBH obtained from the $I-V$ and the photovoltage measurements.

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