Analysis of Schottky Barrier Height in Small Contacts Using a Thermionic-Field Emission Model

Moongyu Jang and Junghwan Lee

This paper reports on estimating the Schottky barrier height of small contacts using a thermionic-field emission model. Our results indicate that the logarithmic plot of the current as a function of bias voltage across the Schottky diode gives a linear relationship, while the plot as a function of the total applied voltage across a metal-silicon contact gives a parabolic relationship. The Schottky barrier height is extracted from the slope of the linear line resulting from the logarithmic plot of current versus bias voltage across the Schottky diode. The result reveals that the barrier height decreases from 0.6 eV to 0.49 eV when the thickness of the barrier metal is increased from 500 Å to 900 Å. The extracted impurity concentration at the contact interface changes slightly with different Ti thicknesses with its maximum value at about 2.9×10^{20} cm^{-3}, which agrees well with the results from secondary ion mass spectroscopy (SIMS) measurements.

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I. INTRODUCTION

The contact between silicon and metal plays an important role in integrated circuit technology. The physics involved in this contact has been interpreted using the Schottky barrier concept. When the doping level in the silicon is low, the Schottky barrier acts as a diode that has a lower turn-on voltage than a p-n junction diode. With this advantage, the Schottky diode has been frequently used in high-speed devices such as those in GaAs [1], [2]. With an increased doping concentration at the interface, the Schottky diode becomes an ohmic contact with severe barrier lowering resulting from an increased tunneling current [3], [4].

Many experimental and theoretical studies of the current flow mechanism in Schottky barriers have been reported [1]-[10]. Crowell and Sze used Schottky's diffusion theory and Bethe's thermionic emission theory to evaluate the Schottky barrier [5]. They included the effects of image force rounding of the barrier and the potential transition from image force to conduction band in the metal. Padovani and Stratton analyzed tunneling currents in Schottky barriers from the standpoint of field and thermionic-field emission using a one dimensional Wentzel-Kramer-Brillouin (WKB) approximation [7]. However, their analysis ignored image force effects and used a simple parabolic barrier shape. The WKB approximation is valid only for smoothly varying potential profiles and, therefore, is not accurate at the top of the barrier [5]. Recently, Sassen, Witzigmann, Wolk, and Brugger analyzed a Schottky diode using the transfer matrix method in GaAs. Their result was expressed as an integral including the transmission coefficient T, which requires numerical analysis [1]. Shenai and

Dutton analyzed a Schottky barrier using image force effects, surface charge density, and the dipole effect, which was modeled as a single exponential decay of the total interface charge. They also considered the series resistance in a Schottky barrier device [2].

The thermionic emission theory applies when the barrier height is much larger than the thermal energy and the current flow depends mainly on the barrier height. In this case, the logarithmic plot of the current with applied voltage gives a linear line, and thus allows easy analysis of the barrier height and ideality factor.

However, as the impurity concentration increases, thermionic-field emission becomes the dominant factor and the current flow depends on both the barrier height and the impurity concentration. In thermionic-field emission, the logarithmic plot of the current with applied voltage deviates from a linear behavior as the tunneling current increases. Note that it is difficult to extract Schottky barrier energy and impurity concentration since the plot is not linear.

To investigate the characteristics of the Schottky diode, three methods—current-voltage measurement, activation energy measurement, and photoelectric measurement—have been widely used [8]. However, for the very small contacts used in deep submicron technology, it is difficult to use activation energy measurement and photoelectric measurement due to area restriction. Therefore, current-voltage measurement is the best method for very small contacts.

In deep submicron metal contacts, the thickness of the barrier metal plays a critical role in contact resistance and leakage current. The Ti/TiN stack layer has been widely used as a barrier metal [11]. However, the Ti thickness is a major factor in the contact resistance since it reacts with silicon, and thus forms $TiSi_2$. The reaction rate between Ti and Si depends on the Ti thickness and doping concentration in the junction. It is not well understood how the Schottky barrier behaves with different Ti thicknesses in a small contact.

In this work, the Schottky barriers of small metal-semiconductor contacts as a function of Ti thickness are estimated using the thermionic-field emission model based on the forward biased current-voltage measurement method.

II. THEORY

The four mechanisms by which carrier transport occurs in Schottky barriers are thermionic emission over the potential barrier, carrier tunneling through the potential barrier, carrier recombination and/or generation in the depletion region, and carrier recombination in the neutral region, which is equivalent to minority-carrier injection. In these mechanisms, the dominant modes of carrier flow in metal-semiconductor contacts are thermionic emission and carrier tunneling [9]. In an ideal metal-semiconductor system, the potential energy barrier to the flow of charge carriers is primarily determined by the work-function difference between the metal and the semiconductor. In practice, however, the barrier height also varies as a function of electric field and impurity concentration at the interface.

Padovani and Stratton assumed a simple parabolic barrier shape by ignoring barrier lowering due to image force and uniform doping. In an intermediate temperature range, where thermionic-field emission is dominant, the current density in the forward direction is expressed by the following equation [7].

$$J = J_S \exp(qV / E_{00}). \tag{1}$$

Ignoring the error function term [7], the saturation current is given as

$$J_S = \frac{A\pi^{1/2} E_{00}^{\ 1/2} \ (E_B - qV + \xi_2)^{1/2}}{kT \cosh(E_{00} / kT)} \exp\left[\frac{\xi_2}{kT} - \frac{E_B + \xi_2}{E_{00}}\right], \tag{2}$$

where E_B is the potential energy of the top of the barrier with respect to the Fermi level of the metal, V is the applied bias between the metal and the semiconductor, ξ_2 is the energy of the Fermi level of the semiconductor measured with respect to the bottom of its conduction band, k is the Boltzmann constant, T is the Kelvin temperature, and A is the classical Richardson constant.

E_{00} is a constant related to the WKB expression for the transmission of the barrier and is given as follows [6].

$$E_{00} = 1.85\times10^{-11} (N/m_r \cdot \varepsilon_r)^{1/2} \text{ eV}, \tag{3}$$

where N is the doping concentration at the metal-semiconductor interface in the unit of cm^{-3}, m_r is the tunneling effective mass measured in the unit of the free electron mass, and ε_r is the relative dielectric constant of silicon.

If the externally applied voltage across the metal-semiconductor is much smaller than the Schottky barrier (i.e., $qV \ll E_B$), the voltage dependency of the saturation current J_S can be ignored and the current density can be expressed as follows.

$$J = J_{S0} \exp(qV / E_{00}), \tag{4}$$

$$J_{SO} = \frac{A\pi^{1/2} E_{00}^{\ 1/2} (E_B + \xi_2)^{1/2}}{kT \cosh(E_{00}/kT)} \exp\left[\frac{\xi_2}{kT} - \frac{E_B + \xi_2}{E_{00}}\right], \tag{5}$$

where J_{S0} is the saturation current without applied voltage.

Note that the logarithmic plot of the current density as a function of the applied bias V gives a straight line of slope q/E_{00}, and from the extracted E_{00}, the impurity concentration can be calculated by (3). Also, the Schottky barrier height E_B can be calculated using (5).

The specific contact resistance R_c, which is an important factor in ohmic contacts, is defined by the following equation [2], [4].

$$R_C \equiv \left(\frac{\partial J}{\partial V}\right)^{-1}_{V=0} = \frac{E_{00}}{q \cdot J_{S0}}. \quad (6)$$

By replacing E_{00} with kT, the expression of R_c in (6) becomes comparable to the result from the thermionic emission model [8].

III. EXPERIMENTAL

We used a 0.25 μm embedded DRAM process to fabricate the metal contact to the p+ junction in N-Well using a p-type <100> silicon substrate with resistivity from 9 to 12 Ω-cm. After formation of the modified LOCOS isolation and gate patterning, a p+ junction was formed by BF_2 implantation with an energy level of 30 keV and a dose of 2.0×10^{15} cm^2. After forming the DRAM cell, we used a CMP process for planarization. After patterning the metal contact by deep UV lithography, we used dry etching to open the contact holes. The metal contact depth was 2.4 μm and the size 0.32 μm × 0.32 μm. Note that the DRAM cell topology caused the deep metal contact. After removing the native oxide in the contact hole using a buffered oxide etchant, we deposited a barrier metal and annealed it at 650 °C for 10 min to form $TiSi_2$ at the metal-semiconductor interface. To investigate the variation of the Schottky barrier's height according to the thickness of the barrier metal, we chose thicknesses for the Ti: 500 Å, 700 Å and 900 Å. We filled the contact hole with tungsten and used aluminum for the metal line.

The contact resistance was measured by the Cross Bridged Kelvin Resistor (CBKR) pattern and the current-voltage characteristics of the contact by a semiconductor parameter analyzer (HP4156A). We investigated the interface morphology between the barrier metal and the silicon junction using transmission electron microscopy (TEM).

IV. RESULTS AND DISCUSSION

Figure 1 shows the logarithmic current-voltage (*I-V*) plot of the manufactured metal-semiconductor contact: closed circles, open squares, and closed diamonds correspond to measured data with Ti thicknesses of 500 Å, 700 Å, and 900 Å, respectively. The current-voltage curve is measured in a CBKR pattern to exclude parasitic resistance components. As the figure shows, the measured log *I-V* curve is not linear. Sze asserted that if thermionic emission is dominant, which is the major current flow mechanism for low impurity concentrations, the curve should be linear [8]. Padovani and Stratton reported that even if thermionic-field emission is dominant, which occurs at a highly doped metal-semiconductor interface, the log *I-V* curve is approximately linear with applied bias voltage [7], while Lepselter and Andrews wrote that if direct tunneling is dominant, the current is directly proportional to the applied bias [10], which implies the ideal ohmic contact. However, our result in Fig.1 indicates that the *I-V* characteristics of the contact do not follow the behavior of any of these three models.

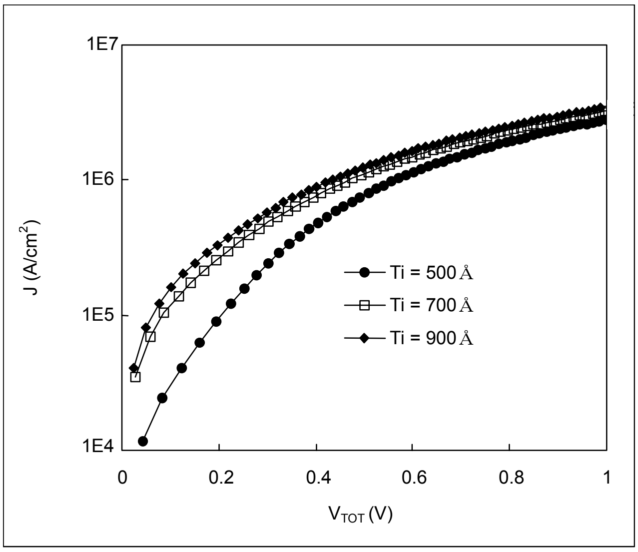

Fig. 1. *I-V* characteristic curve of the metal-semiconductor contact in a highly doped p^+ junction. The contact hole size is 0.32 μm×0.32 μm. Closed circles, open squares, and closed diamonds represent data with Ti thicknesses of 500 Å, 700 Å, and 900 Å, respectively.

Figure 2 shows the voltage dependence of the contact resistance. The components of the contact resistance can be divided into two parts: the Schottky diode and the spreading resistance caused by current crowding that is due to the small size of the contact. The non-linear behavior depicted in Fig. 1 is caused by spreading resistance, which is negligible in relatively larger contacts.

In Fig. 2, the resistance approaches 220 Ω, irrespective of the thickness of the barrier metal, as the applied bias voltage increases. This is likely related to current crowding in a small contact hole as reported in [2] and [11]. As mentioned, the total resistance across the contact consists of R_{di} caused by the Schottky diode and R_{sp} caused by spreading resistance as the inserted equivalent circuit in Fig. 2 explains. Note that R_{di} depends on the applied voltage, while R_{sp} depends not on applied voltage, but on contact size and doping level. Hence, as the voltage difference between the V_H and V_L nodes increases, R_{di} approaches zero because of the increased thermionic-field emission and the total resistance is identical to R_{sp}. Therefore, from the results of Fig. 2, we can deduce that R_{sp} is 220 Ω.

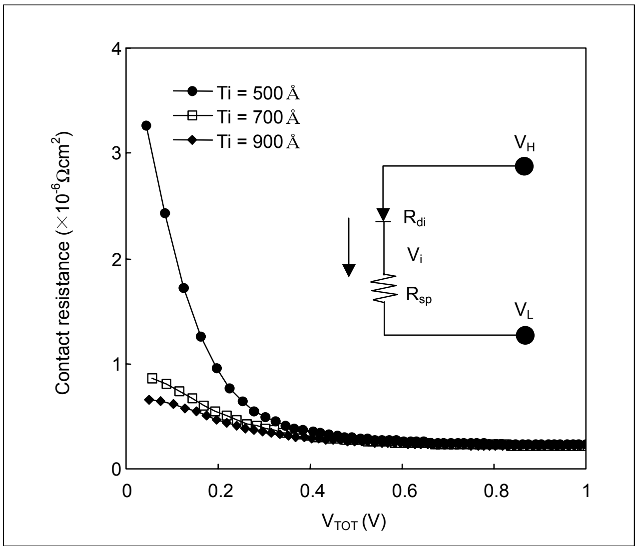

Fig. 2. The variation of contact resistance with applied bias across the Kelvin resistor. The contact hole size is 0.32 μm × 0.32 μm. Closed circles, open squares, and closed diamonds represent data with Ti thicknesses 500 Å, 700 Å, and 900 Å, respectively. The insert represents the equivalent circuit of the resistor in a CBKR pattern assuming that the Schottky diode and spreading resistor is serially connected. R_{di} denotes the resistance of the Schottky diode and R_{sp} denotes the spreading resistance. V_H-V_L corresponds to the externally applied bias voltage across the Kelvin resistor and V_i represents the voltage between the Schottky diode and spreading resistor.

The effect of barrier metal thickness is clearly shown in Fig. 2. The specific contact resistance, which is the contact resistance at zero bias voltage, increases abruptly at a Ti thickness of 500 Å. This is probably because not enough $TiSi_2$ formed at the interface due to the very deep contact height and small contact size, which resulted in an increase of the Schottky barrier height at a Ti thickness of 500 Å. In fact, the TEM images of the contacts with different Ti thicknesses clearly show that the $TiSi_2$ layer formed with a Ti thickness of 500 Å is not uniform and has a relatively much thinner $TiSi_2$ layer in some parts (Fig. 3). Note that the formed $TiSi_2$ layers are very uniform when the Ti thickness exceeds 700 Å.

Figure 4 shows the dependency of the voltage drop across the Schottky diode (V_{di}) and spreading resistance (V_{sp}) as a function of the applied voltage for a Ti thickness of 500 Å. The closed and open circles correspond to the voltage applied across the Schottky diode (V_{di}) and the spreading resistor (V_{sp}), respectively. It appears that V_{di} saturates at 0.375 V, while V_{sp} increases linearly as the total applied bias increases. The figure shows clearly that the ohmic characteristic is achieved when the applied voltage between the V_H and V_L node exceeds 0.75 V.

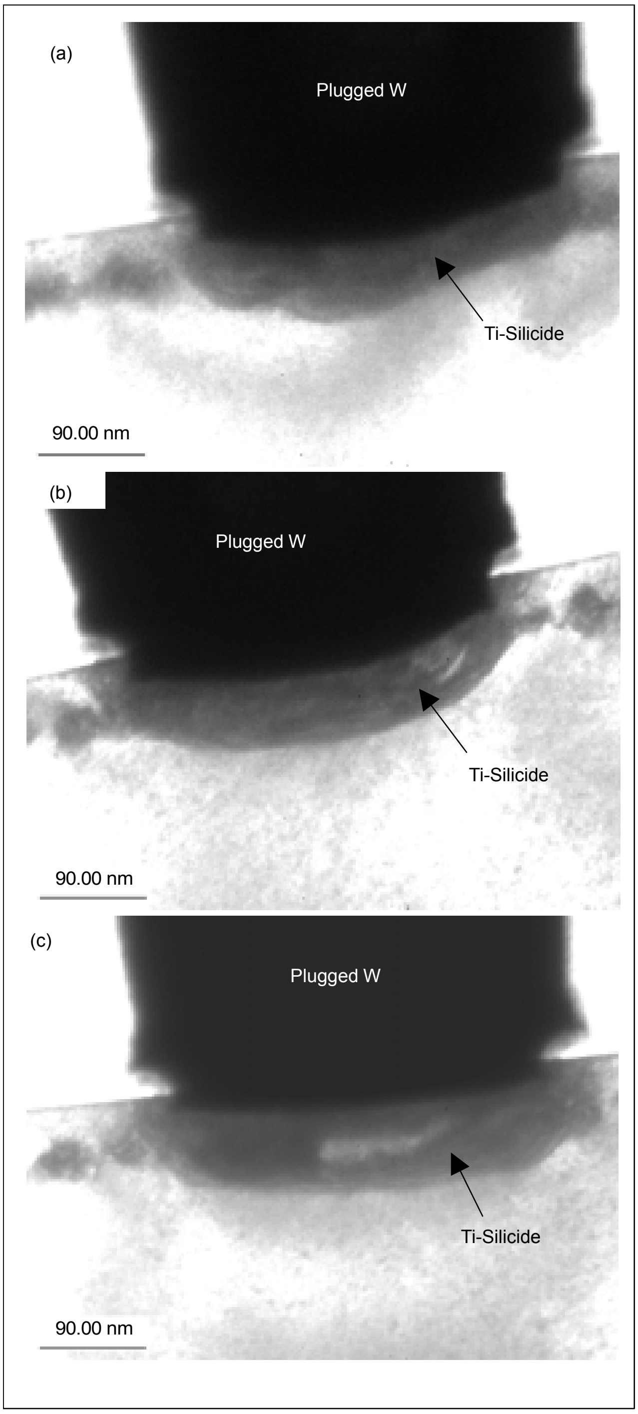

Fig. 3. TEM images of metal-semiconductor interface. (a), (b), and (c) represent images with thicknesses 500 Å, 700 Å, and 900 Å, respectively.

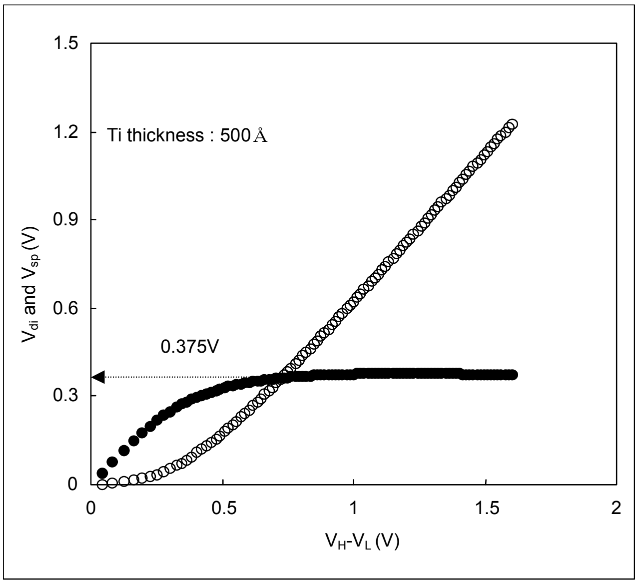

Fig. 4. The voltage components in CBKR for 500 Å Ti. Closed and open circles represent the voltage component biased across the Schottky diode (V_{di}) and spreading resistor (V_{sp}), respectively.

To accurately analyze the thermionic-field emission model, the net applied voltage across the Schottky diode (V_{di}) should be used instead of the total applied bias across the CBKR pattern (V_H-V_L), since the CBKR pattern does not give a linear relationship in the logarithmic plot of the current to the total applied voltage, as discussed in relation to Fig. 1.

Figure 5 shows the logarithmic plot of the current as a function of V_{di} at different Ti thicknesses. Closed circles, open squares, and closed diamonds represent the measured data for Ti thicknesses of 500, 700, and 900 Å, respectively. It appears that the plots in Fig. 5 are linear, while the logarithmic plot of the current as a function of the total applied voltage deviates from the linear line as shown in Fig. 1. We used the least square fitting method for straight lines to extract E_{00} and J_{S0}. The logarithmic linear dependency of the current on the net bias voltage across the Schottky diode (V_{di}) strongly supports the validity of our assumption of voltage dependency in J_S and the use of (5). In Fig. 5, E_{00} is calculated from the slope, while J_{S0} is obtained from the intersection of the Y-axis. With the extracted E_{00} and J_{S0}, the impurity concentration N, Schottky barrier height E_B, and specific contact resistance R_c are calculated by applying (3), (5), and (6), respectively.

Table 1 summarizes the extracted parameters. In the calculation of the Schottky barrier height E_B and impurity concentration N, the effective tunneling mass (m_r) for the hole, the Richardson constant (A) for the <100> p-type substrate, and the relative dielectric constant (ε_r) are assumed as 0.9163, 79 Acm^{-2} K^{-2}, and 12, respectively [4], [12], [14]. It appears that the extracted Schottky barrier height decreases from 0.60 eV to 0.49 eV when the Ti thickness increases from 500 Å to 900 Å. The higher Schottky barrier height for the 500 Å Ti thickness may come from the imperfect formation of $TiSi_2$ deduced from the irregular interface morphology in Fig. 3. Typically, in a low doped Schottky diode, the barrier height of p^+ is about 0.70 eV [8]. However, the barrier height is lowered in a highly doped p^+ junction due to the image charge and tunneling. If the impurity concentration is 10^{20} cm^{-3}, the calculated depletion width is about 28 Å and the barrier lowering by the image charge is 0.225 eV [2], [8]. When the barrier lowering in a highly doped p^+ junction is considered, the extracted Schottky barrier height is comparable to the results of previous work [8], [13]. Table 1 reveals that the extracted maximum concentration of impurity is about 2.9×10^{20} cm^{-3}, which is comparable to our secondary ion mass spectroscopy (SIMS) result (Fig. 6).

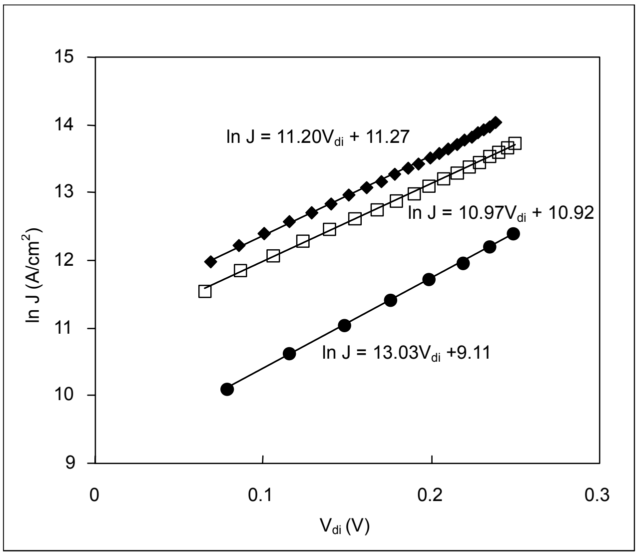

Fig. 5. The logarithmic plot of current with net bias voltage applied across the Schottky diode (V_{di}). Closed circles, open squares, and closed diamonds represent data with Ti thicknesses of 500 Å, 700 Å, and 900 Å, respectively.

Table 1. Summary of extracted parameters.

Ti thickness [Å]	E_{00} [eV]	J_{S0} [A-cm^{-2}]	R_c [Ω-cm^2]	N [cm^{-3}]	E_B [eV]
500	0.0767	9.08E3	5.09E-6	2.06E20	0.60
700	0.0911	5.51E4	9.98E-7	2.91E20	0.53
900	0.0893	7.83E4	6.83E-7	2.80E20	0.49

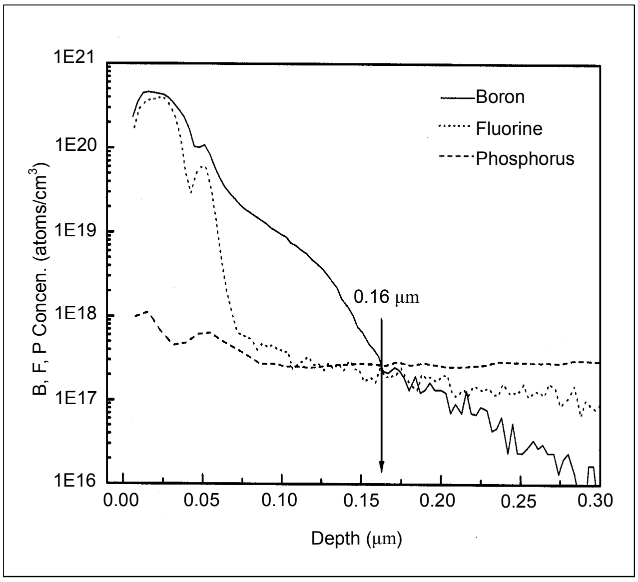

Fig. 6. The SIMS profile of the p+ junction.

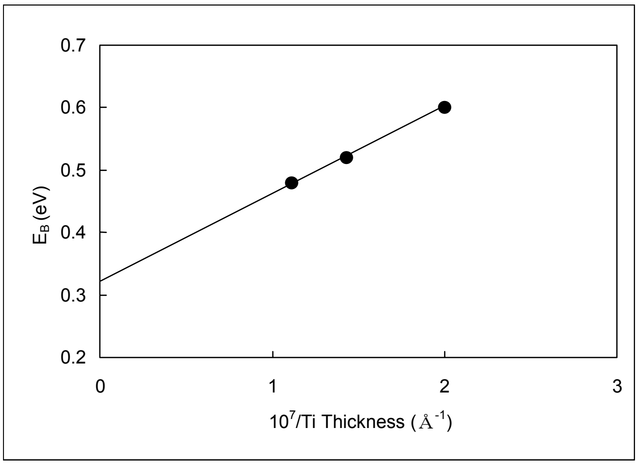

Fig. 8. The dependence of Schottky barrier height to Ti thickness, which clearly shows an inversely proportional characteristic. From this graph, the minimum achievable Schottky barrier height can be estimated with Ti thickness.

Figure 7 shows the logarithmic plot of specific contact resistance (R_c) versus E_B /sqrt(N), which validates the analysis in this work. In the region dominated by thermionic-field emission and direct tunneling, the variation of the logarithmic specific contact resistance with E_B/sqrt(N) should be linear as shown in [3], [8]. The linear variation indicates that the major current flow mechanism is thermionic-field emission. The figure also indicates that the specific contact resistance can be reduced by up to 10% if the barrier height and impurity concentration are optimized.

Figure 8 shows the variation of the Schottky barrier as a function of Ti thickness. As shown, the Schottky barrier is inversely proportional to the Ti thickness. Note that the minimum barrier height is 0.33 eV with unlimited Ti thickness.

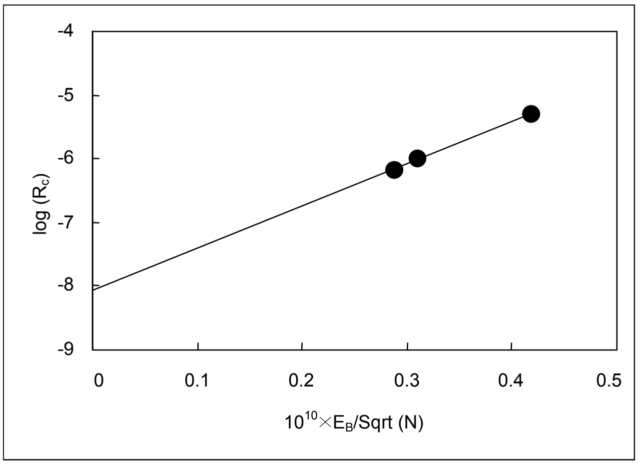

Fig. 7. The log(R_c) versus E_B/sqrt(N) graph. In thermionic-field emission and direct tunneling dominant region, the graph shows linear behavior.

However, the junction leakage current increases as the barrier metal thickness increases because of excessive Ti atoms. From our experiments, 900 Å of Ti is optimal in terms of contact resistance and junction leakage.

V. CONCLUSION

We used current-voltage measurements to extract the Schottky barrier height of small contacts. The metal-semiconductor contact in a highly doped junction shows non-ideal diode curves, which is caused by spreading resistance. Therefore, we extracted the net applied bias voltage across the Schottky diode by assuming a serial connection between the Schottky diode and the spreading resistor. It appears that when the net bias voltage is applied across the Schottky diode, the *I-V* curves follow the thermionic-field emission model. Using this model, we extracted the Schottky barrier height and impurity concentration. Our investigation revealed that the barrier height decreased from 0.6 eV to 0.49 eV when the thickness of the barrier metal was increased from 500 Å to 900 Å. The extracted impurity concentration at the contact interface changed slightly with a changing Ti thickness with its maximum value at about 2.9×10^{20} cm^{-3}, which is in good agreement with the result from our SIMS measurement.

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