A Self-Consistent Characterization Methodology for Schottky-Barrier Diodes and Ohmic Contacts

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***Abstract*— Based on the simple interfacial-layer theory, the extraction methods for the interface parameters of the metal-semiconductor contact have been developed and applied to characterize both the Schottky-barrier diodes and the ohmic contacts in a self-consistent manner. It has been shown that the physical parameters at the metal-semiconductor interface can be extracted from the I-V characteristics of the Schottky-barrier diodes and the degradation of the thermal-equilibrium barrier height due to the thermal cycle can be directly modeled in terms of the extracted interface parameters. Besides, using the extracted parameters, the specified surface-treatment process can be evaluated by the extracted thermal-equilibrium barrier height, and thus the strongly process-dependent specific contact resistivity ρ_c of the ohmic contacts can be theoretically calculated by a modified tunneling model considering the impurity band. Furthermore, by comparing the simulated results and the measured ρ_c data deduced from the Al and Ti contacts on both doping types of the Si-substrate, satisfactory agreements have been obtained.**

I. Introduction

In modern MOS/VLSI fabrication technology, both the rectifying and ohmic contacts are important [1]–[2]. In order to reduce the parasitic series resistance and thus to enhance the performance of submicrometer devices, the specific contact resistivity ρ_c of the ohmic contacts should be properly controlled. When the experimental ρ_c data are compared to the theoretical results generated by the tunneling theory [3]–[5], three basic parameters governing the contact resistance should be carefully determined, e.g., surface doping concentration N_S, tunneling effect mass m_t^*, and Schottky-barrier height. In order to compare the experimental ρ_c data with the theoretical results, the tunneling effective mass or/and the Schottky-barrier height [4]–[5] are often treated as the fitting parameters. Moreover, it is quite unsuitable to adopt the Schottky-barrier height from the literatures without considering their detailed fabrication procedures. It should be emphasized that different fabrication procedures will contribute to different interface properties and thus different Schottky-barrier heights for the metal/semiconductor (M/S) contacts even using the same contact metal. Furthermore, in the existing VLSI fabrication process, the diode ideality factor is often found to be much deviated from unity. This fact imposes another difficulty on accurately determining the Schottky-barrier height. Therefore, as the surface doping concentration of the ohmic contacts is not significantly degraded after the processes of metal deposition and thermal treatments, the appropriate determination of the Schottky-barrier height seems to be the first and most crucial step for characterizing the ohmic contacts. In the present studies, the most frequently used experimental methods to characterize the interface states are the Schottky capacitance spectroscopy (SCS) [6]–[7] and the newly developed current-voltage (I-V) method [8]. Although the density distribution of the interface states and their associated interface properties have been obtained by using any of these proposed methods, their relations with the thermal-equilibrium barrier height and their effects on the formed ohmic contacts have not been made until now.

In this paper, the interface effects on the Schottky-barrier diodes and the ohmic contacts have been characterized both theoretically and experimentally in a self-consistent manner. Experiments have been performed by depositing Al and Ti metals on both n-type and p-type Si substrates to fabricate the Schottky-barrier diodes and the Cross Bridge Kelvin Resistor (CBKR) at the same time. Using the developed interfacial-layer theory with considering the density distribution of the interface states within the energy gap, the interface parameters are deduced from the I-V characteristics of the fabricated Schottky-barrier diodes. It has been shown that the thermal-equilibrium barrier height can be well modeled in terms of the extracted interface parameters and its dependence on the fabrication process can be further evaluated by considering the dominant type and the density distribution of the interface states. Besides, excellent agreements between the experimental results and the theoretical calculations for ρ_c have been obtained, which support the physical validity of our proposed model and characterization method.

II. Theory

A. Thermal-Equilibrium Barrier Height

It is assumed that the interface states are spatially localized within the bandgap, and their charging behaviors are highly dependent on the bias condition. If the occupation function f_{it} for both the acceptor-like and donor-like interface states are indistinguishable, the net charge density trapped in the

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interface states can be expressed as

$$Q_{it}(V_S) = -q\int_{Ev}^{Ec} D_{it}(E)f_{it}(E,V_S)dE + q\beta\int_{Ev}^{Ec} D_{it}(E)dE \quad (1)$$

where $D_{it}(E) = D_{it}^a(E)+D_{it}^d(E)$ is the sum of both types of the interface-state densities; β is used to quantitatively specify the ratio of the density of the donor-like interface states to the total density of the interface states and is expressed by

$$\beta = \int_{Ev}^{Ec} D_{it}^d(E)dE \Big/ \int_{Ev}^{Ec} D_{it}(E)dE. \quad (2)$$

Considering a metal/n-type semiconductor Schottky-barrier contact with the interfacial layer, the potential drop across the interfacial layer at thermal equilibrium Δ_0 can be written as [9]

$$\Delta_0 = [Q_{sc}(0) + Q_{it}(0)]/C_i \quad (3)$$

where $C_i\ (= \epsilon_i/\delta)$ is the interfacial-layer capacitance, and Q_{sc} is the space-charge density in the surface depletion region, which can be expressed as

$$Q_{sc}(V_S) = [2q\epsilon_s N_D(\phi_{bn,0} - V_n - V_S - V_t)]^{1/2} \quad (4)$$

where $\phi_{bn,0}$ is the thermal-equilibrium barrier height; V_n is the potential difference between the Fermi level and the conduction band edge in the neutral region; V_S is the potential drop across the semiconductor surface depletion layer; V_t is the thermal voltage; and N_D is the doping concentration of the lightly-doped substrate.

A relationship among the metal work function ϕ_m, the electron affinity χ, and $\phi_{bn,0}$ is given as

$$\phi_m - \chi = \phi_{bn,0} + \Delta_0. \quad (5)$$

Using (1)–(5), $\phi_{bn,0}$ can now be solved using the iteration method. The calculation of $\phi_{bn,0}$ shows that the thermal-equilibrium barrier height of the M/S junction is strongly influenced by the interface states in the semiconductor band gap. For a Schottky-barrier diode fabricated on a lightly-doped semiconductor, the thermal-equilibrium barrier height is nearly independent of doping concentration. Figs. 1(a) and (b) show the dependence of $\phi_{bn,0}$ on $\phi_m - \chi$ and β for a constant interface-states distribution with the density of states $D_{it,0}$, respectively. Since $\phi_{bn,0}$ is very sensitive to $D_{it,0}$ which is a strongly process-related factor, different Schottky-barrier heights have been reported for the Schottky-barrier diodes fabricated by the same contact metal. Moreover, as $D_{it,0}$ increases beyond a certain quantity, $\phi_{bn,0}$ will saturate to a constant value and is independent of the kinds of the contact metal, as shown in Fig. 1(a). Furthermore, the saturation value for $\phi_{bn,0}$ is strongly influenced by the physical parameter β which specifies the controllability of the type of the interface states through the net charge density, as shown in Fig. 1(b). For the uniformly distributed interface states, the saturation value of $(1-\beta)E_g/q$ is obtained, in which the term of $\beta E_g/q$ is just equivalent to the neutral level ϕ_0 [9].

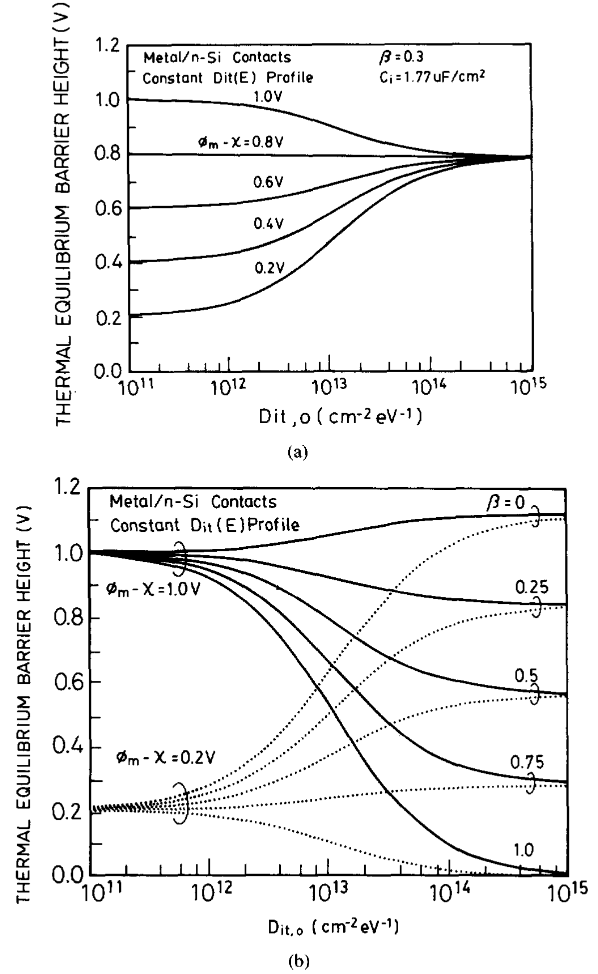


Fig. 1. $\phi_{bn,0}$ as a function of $D_{it,0}$ with (a) $\phi_m - \chi$, and (b) β as a variable.

Accordingly, the pinning of the Fermi-level at the interface by the sufficiently large interface-state density depends on the most active type of the interface states. We assume that β is strongly dependent on the process-related factors in addition to the specified properties of the semiconductor. Therefore, a negligible discrepancy among the measured barrier heights is not sufficient to conclude the permanence of the surface properties because different values of $D_{it,0}$ and β for the same $\phi_m - \chi$ can result in the similar barrier height, as shown in Fig. 1(b). This fact is especially emphasized because the barrier height has been widely applied to study the effects of either physical damages or chemical reactions on the M/S contacts.

B. Characterization of the Interface Properties

The majority-carrier density J_n for a Schottky-barrier diode fabricated on the n-type substrate can be obtained by using the

interfacial layer-thermionic emission-diffusion theory [10]:

$$J_n = \frac{\theta_n A_n^{**} T^2}{1 + \theta_n \dfrac{\nu_{rn}}{\nu_{dn}}} \text{EXP}\left(-\frac{q\phi_{bn,0}}{k_b T}\right) \text{EXP}\left(-\frac{qV_i}{k_b T}\right) \cdot \left[\text{EXP}\left(-\frac{qV}{k_b T}\right) - 1\right] \quad (6)$$

where θ_n is the transmission coefficient of electrons across the interfacial layer; A_n^{**} is the modified Richardson constant for electrons; $\nu_{rn} = A_n^{**}T^2/qN_c$ is the thermal velocity in the current-flow direction for electrons; and ν_{dn} is the effective diffusion velocity associated with the transport of electrons. The forward bias V can be divided into two components, i.e., $V = V_S + V_i$, where V_i is the potential drop across the interfacial layer and V_S is that across the semiconductor surface depletion layer. V_i can be expressed as [10]:

$$V_i = [Q_{sc}(0) + Q_{it}(0) - Q_{sc}(V_S) - Q_{it}(V_S)]/C_i. \quad (7)$$

According to this relation, it is clearly seen that the voltage drop across the interfacial layer can not be neglected if the interface effects become important, e.g., when C_i is decreased and the variation of Q_{it} becomes prominent. If we adopt the definition of the "diode ideality-factor" n as $(q/k_bT)(dV_f/dln(I_f))$ in the low current level, using (6) and (7) we obtain:

$$n \approx \left[1 - \frac{1}{C_i}\left(\frac{dQ_{sc}}{dV_f} + \frac{dQ_{it}}{dV_f}\right)\right]^{-1}. \quad (8)$$

Therefore, the nonideality of the I-V characteristics is mainly caused by the charge variations due to the interaction between the interface states and the electrons in the semiconductor.

According to (6) and (7), the physical parameters, such as $\phi_{bn,0}$ and C_i, can be extracted from the measured reverse I-V characteristics since the net charge trapped in the interface states is kept unchanged under the reverse bias. The possibility of extracting C_i and $\phi_{bn,0}$ from the soft reverse I-V characteristics is based on the theoretical studies on the charging behavior of the interface states which are in equilibrium with the semiconductor using the Shockley–Read–Hall (SRH) statistics. The net charges residing in the interface states will quickly go to a constant value if the applied reverse-bias voltage increases beyond a certain value, e.g., 1 V. The conclusion has been confirmed by the C-V measurement that no extra capacitance due to the charge-density variations in the interface states can be observed for a reversely biased Schottky-barrier diode. Moreover, by substituting the extracted $\phi_{bn,0}$ and C_i into (6) and comparing with the measured forward I-V characteristics, $D_{it}(E)$ can be numerically obtained if the occupation function of the interface states is completely controlled by the majority carriers at the semiconductor surface under the forward bias [8]. Many reported data [11]–[13] have indicated that the distribution of the interface states across the silicon bandgap exhibits the peaks near both the band edges with a pronounced minimum at the center of the forbidden region. Therefore, the experimentally observed density profile can be generally described by a double-peaked distribution:

$$D_{it}(E) = D_{it,0}\left\{\text{EXP}\left[-\left(\frac{E - E_1}{\sqrt{2}\Delta E}\right)^2\right] + \text{EXP}\left[-\left(\frac{E - E_2}{\sqrt{2}\Delta E}\right)^2\right]\right\} \quad (9)$$

where E_1 is the peak energy level above the valence band E_V; E_2 is the other peak level equal to $(E_g - E_1)$ with the reference energy level at E_V; ΔE is the standard energy deviation of the interface-state density; and $D_{it,0}$ is the maximum density at E_1 and E_2. Therefore, the measured $D_{it}(E)$ was fitted by assuming E_1 above E_V of 0.1 eV and 0.21 eV for Al and Ti contacts, respectively [14]. The fitted $D_{it}(E), \phi_{bn,0}$, and C_i were then applied to solve the physical parameter β. Since the interface properties were assumed to be not altered by the insertion of the implanted layer, the physical parameters deduced from the Schottky-barrier diodes together with N_S and m_t^* can be used to generate ρ_c. The flowchart showing the extraction and the computation procedures for these physical parameters is shown in Fig. 2.

Note that the presence of an interfacial dielectric layer, e.g., the native SiO_2 layer, is not the necessary condition for the use of the interfacial layer-thermionic-diffusion theory. Any structural transition layer consisting of the structure defects varied their local bonding configuration after metal deposition can be recognized as the interfacial layer. This layer is radically different from the predeposited one and may be caused by the strain field released by either the lattice or the grain boundary mismatch at the M/S interface. In fact, the metal-silicon interdiffusion and reaction may occur even at room temperature, which will result in an interfacial layer with different characteristics from that before metal deposition. Thus, the extracted interfacial layer capacitance can be used to describe the interface reconstruction after the formation of the M/S junction. Moreover, our proposed characterization method can be applied to study any process-related effect on the M/S contacts even their interface structures are strongly degraded after processing [15].

C. Specific Contact Resistivity

In our study, several assumptions have been made for the physical properties of the ohmic contacts: 1) the thermal-equilibrium barrier height is kept unchanged both on the lightly and heavily doped substrates if these M/S contacts are simultaneously processed. That is, the surface properties of the semiconductor are mainly dependent on the pre- and post-metal deposition treatments but not on the doping concentration. 2) For a heavily doped semiconductor formed by ion-implantation, the implantation damages can be fully eliminated after the thermal activation procedure. This assumption will ensure that the physical parameters extracted from the Schottky-barrier diodes can be directly applied to simulate the interface properties of the ohmic contacts. 3) Due to the strong interactions either among the introduced impurities themselves or with the host lattice atoms on a heavily doped semiconductor, the discrete energy level broadens into a band,

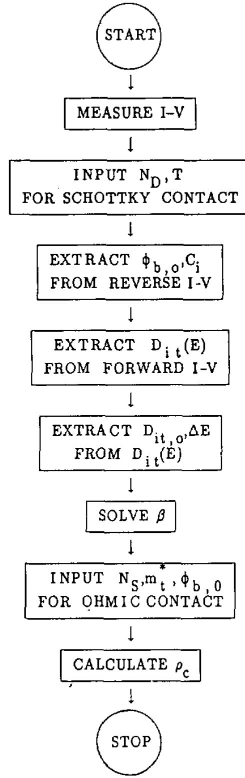
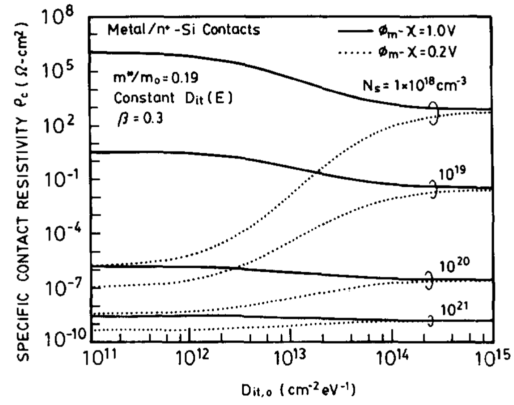
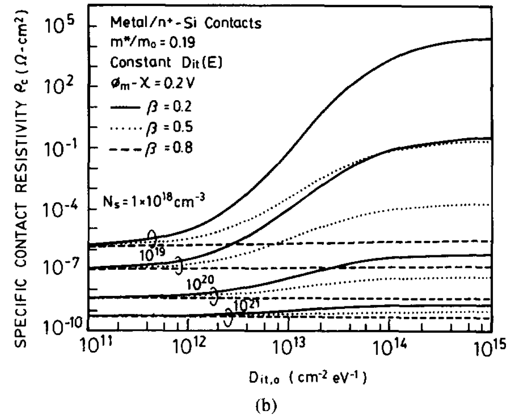


Fig. 2. Flowchart showing the characterization procedures for extracting the interface parameters.



(a)



(b)

Fig. 3. ρ_c as a function of $D_{it,0}$ with (a) $\phi_m - \chi$, and (b) β as a variable.

and the band tail on the band edge falls gradually into the energy gap. Therefore, on calculating the tunneling current for the ohmic contact, the high-doping effects on the density of states which determines the available carriers for the tunneling process can not be neglected. 4) The WKB approximation can be used to calculate the carrier tunneling probability. In general, comparing the tunneling probability calculated from the Schroedinger equation, this approximation provides an acceptable accuracy when the surface concentration of the heavily-doped substrate N_S is higher than 10^{17} cm^{-3} [5].

For a heavily doped M/S contacts, the transport current is dominated by the tunneling process, which can be expressed as [16]

$$J_t = \int_{E_c'}^{E_c'+qV_b} qv_x[F_s(E) - F_m(E)]T_t(E_x)D(E)dE \quad (10)$$

in which V_b is the built-in voltage; v_x is the carrier velocity in the direction of transport; F_s and F_m are the Fermi–Dirac distribution for semiconductor and metal, respectively; $D(E)$ is the effective density of states including the impurity band and the band-edge tailing for a heavily doped semiconductor; and E_c' is the effective conduction band edge which is defined at the energy level above which 90% of the carrier population can be obtained. Due to the high-doping effects, $D(E)$ shows a serious departure from the conventionally used square-root law for a parabolic band, and the electron population and hence the tunneling current for the impurity band is quite different from that for the parabolic band. Details of the calculating procedure are described in the appendix.

T_t is the transmission probability for a quasi-free electron with the energy E_x in the tunneling direction. Note that E_x is measured from the potential minimum at the depletion edge. By using the WKB approximation, T_t can be expressed as [3]–[5]

$$T_t(E_x) = \exp\left\{\frac{-1}{E_{00}}\left[(qV_b)^{1/2}(qV_b - E_x)^{1/2} - E_x \ln\frac{(qV_b)^{1/2} - (qV_b - E_x)^{1/2}}{E_x^{1/2}}\right]\right\} \quad (11)$$

where E_{00} can be expressed as

$$E_{00} = \frac{q\hbar}{2}\left(\frac{N_S}{m_t^* \epsilon_s}\right)^{1/2} \quad (12)$$

in which ϵ_s is the dielectric permittivity of the semiconductor.

The specific contact resistivity is defined as

$$\rho_c = \left(\left.\frac{\partial J_t}{\partial V}\right|_{V=0}\right)^{-1}. \quad (13)$$

When $\phi_m - \chi, C_i$, the dominant type of the interface states β, and the total density distribution of interface states $D_{it}(E)$

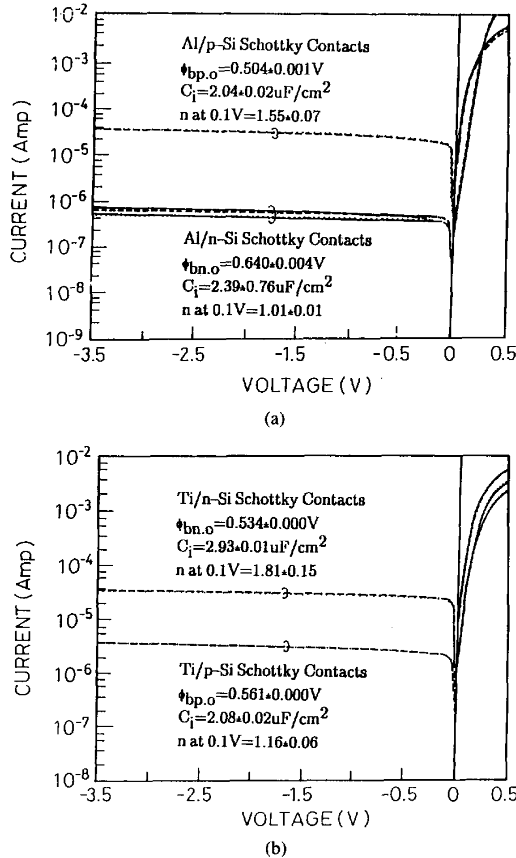


Fig. 4. The measured I-V characteristics for (a) Al/Si and (b) Ti/Si Schottky contacts.

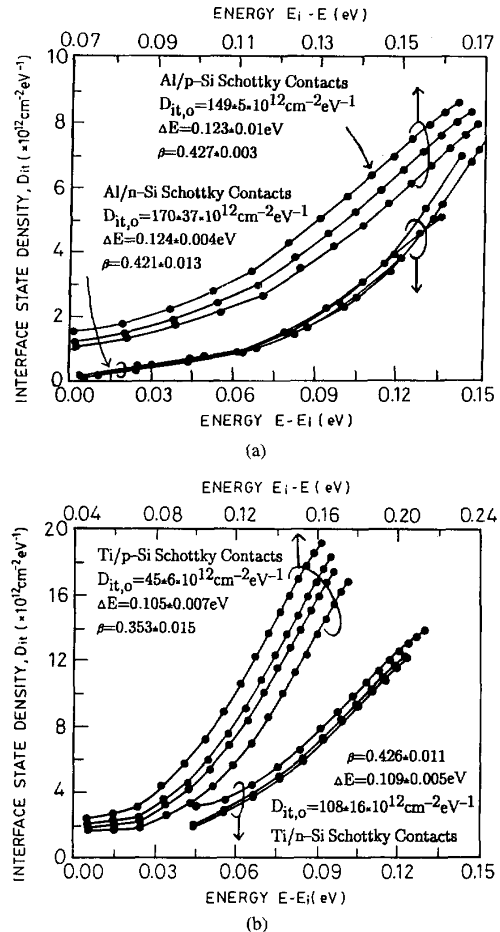


Fig. 5. The measured ISAS for (a) Al/Si and (b) Ti/Si Schottky contacts.

are given, ρ_c can be calculated. As shown in Fig. 1, $\phi_{bn,0}$ is strongly dependent on the interface parameters, such as $\phi_m - \chi, C_i, D_{it,0}$, and β. The sensitivity of the contact plot on these interface parameters is thus further enhanced because the specific contact resistivity ρ_C is an exponential function of $\phi_{bn,0}$ as predicted by the conventionally used tunneling theory. The effects of $\phi_m - \chi, \beta$, and $D_{it,0}$ on ρ_c are shown in Figs. 3(a) and 3(b) for a constant density distribution of the interface states. As shown in Fig. 3(a), ρ_c is less dependent on $\phi_m - \chi$ when N_S becomes strongly degenerate as predicted in the previous studies [4]–[5]. This behavior also occurs when $D_{it,0}$ increases even the substrate is not a heavily doped one. It is important to point out that a large amount of surface damage, which is the main generation source for the interface states, can be introduced either during opening of the contact holes by the dry-etching method or due to the improper post-thermal annealing treatments. Thus the near independence of ρ_c on the types of metal can be expected. Moreover, although m_t^* for n-type and p-type substrates is different and $\phi_{bp,0}$ is usually less than $\phi_{bn,o}, \rho_c$ measured from a p-type ohmic contact may exceed that of a n-type contact when $D_{it,0}$ increases beyond a critical level. Since the strongly process-dependent parameter β plays an important role on $\phi_{bn,0}, \rho_c$ is influenced by β, as shown in Fig. 3(b). The variation of β results in different values for ρ_c even at the same N_S, and the dependence of ρ_c on N_S deviates from the predicted results obtained from the conventional tunneling theory, i.e., $\rho_c \sim \exp(N_S^{-1/2})$. This is the reason why a substantial difference among the experimental ρ_c versus N_S data exists in the published literature even using the same contact metal deposited on a semiconductor with similar doping concentration.

III. Experimental and Theoretical Comparisons

(100)-oriented n^-/n^+ and p^-/p^+ Si epi-wafers with the resistivity of 4–10 Ω-cm for the epi-layer layer were used to fabricate the Schottky-barrier diodes. The other nonepi-wafers were also prepared to fabricate the self-aligned cross bridge Kelvin resistor (CBKR) [17], on which SiO_2 of 4000 Åwas initially grown. The first mask was used to define the horizontal diffusion bar by etching SiO_2 of 2500 Å. The vertical diffusion bar was subsequently defined using the second mask also by etching SiO_2 of 2500Å. The contact window was now automatically exposed at the overlap area of the two diffusion taps, and SiO_2 of 1500 Å was left over the diffusion strips. The first ion implantation was performed with the energy optimized to penetrate SiO_2 of 1500 Å in order

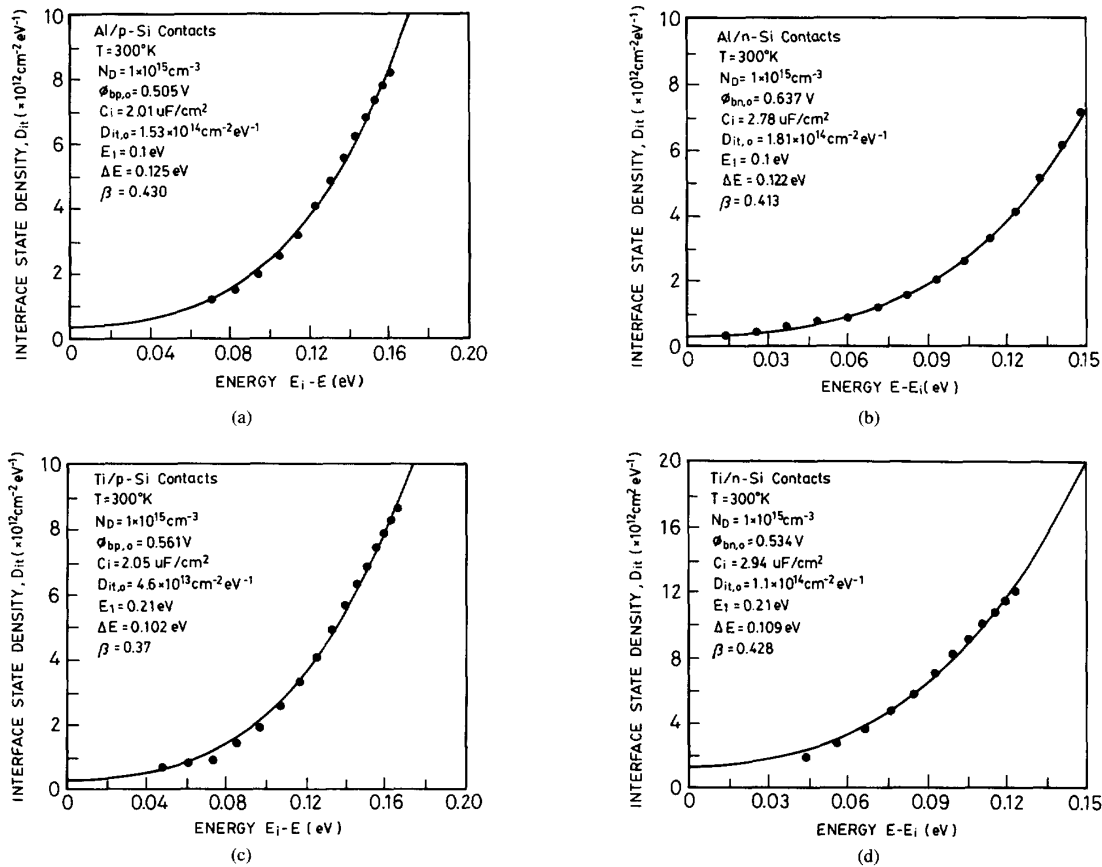


Fig. 6. The measured ISAS and the fitted double-peaked profile for (a) Al/p-Si, (b) Al/n-Si, (c) Ti/p-Si, and (d) Ti/n-Si Schottky contacts.

to provide enough dopants for the conduction channels. The second ion implantation was then done to form the heavily-doped n^+ and p^+ contact region by using As^+ and BF_2^+. The self-aligned CBKR was annealed at 900°C in the N_2 ambient, in which the diffusion tap to the contact overlap was reduced to the level of the lateral dopant diffusion. Prior to loading into the vacuum system, the Schottky and the ohmic contacts received the same surface treatment in a diluted HF solution. Ti and Al were deposited by an E-gun evaporator. The I-V characteristics were measured by a HP4145B pA meter, and ρ_c was deduced from a plot of the contact resistance versus the contact area. Moreover, the surface doping concentration was determined by SRP measurement.

Typical I-V characteristics obtained from different Schottky-barrier diodes on both types of the Si-substrate are shown in Figs. 4(a) and 4(b) for the Al/Si and Ti/Si contacts, respectively. Apparently, a wide range of ideality-factor n varying from 1.01 to 1.96 was deduced, which casts doubt on the accuracy in determining the Schottky-barrier height by using the conventional extrapolation method from the forward I-V characteristics. The nonideality of the I-V characteristics is further analyzed by using the developed interfacial-layer model. The extracted thermal-equilibrium barrier height $\phi_{bn,0}$ (or $\phi_{bp,0}$) and the interfacial-layer capacitance C_i for these diodes are listed in Fig. 4. These two quantities are then applied to extract the interface-state-apparent-spectra (ISAS) from the forward I-V characteristics. Figs. 5(a) and 5(b) show the measured ISAS from various diodes simultaneously fabricated on both types of the Si-substrate for the Al/Si and Ti/Si contacts, respectively. It is clearly seen from these figures that the shape and magnitude are quite different. According to (8), the observed fluctuation of the ideality factor n for the Al and Ti contacts can be attributed to the changes of both the apparent interface-state density measured at $V_f = 0.1$ V and the interfacial-layer capacitance.

Note that the large ideality factor and the soft reverse characteristics can also be explained by considering the inhomogeneities at the M/S interface [18], [19]. However, based on our interfacial layer theory considering the nonequilibrium occupancy of the interface states, the thermal equilibrium barrier height, the soft reverse I-V characteristics, and the nonideality of the forward I-V as well as C^{-2}-V characteristics, can be self-consistently interpreted in an unified manner. Moreover, the effects of a specified process on the Schottky and ohmic contacts can be further predicted because different processes will contribute different interface properties which can be evaluated by using our developed characterization method.

Furthermore, by tuning the values of $D_{it,0}$ and ΔE in (9), the ISAS can be well fitted by a double-peaked profile. Comparisons between theoretical and experimental results are

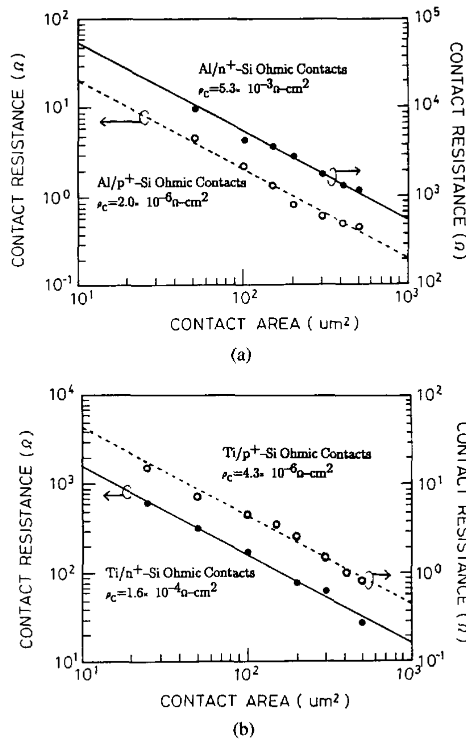


Fig. 7. The measured contact resistance versus the contact area for (a) Al/p$^+$(n$^+$)-Si and (b) Ti/p$^+$(n$^+$)-Si ohmic contacts.

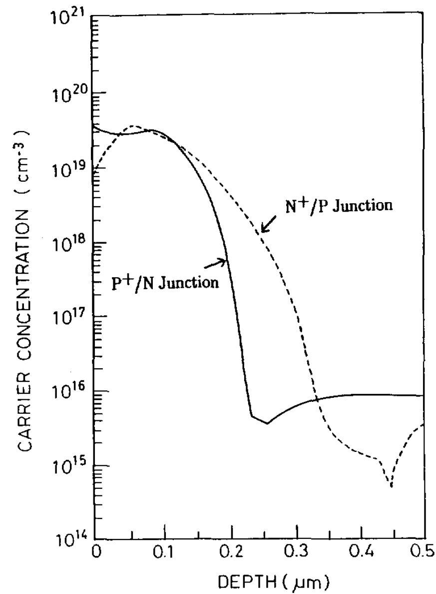


Fig. 8. The spreading resistance profile for p^+/n and $n + /p$ junctions.

shown in Figs. 6(a)–6(d) for the Al and Ti contacts on both types of the substrate. Although the measured ISAS data are quite different, however, they can be well simulated by the proposed profile. The physical parameter β is then solved using $\phi_m - \chi$ of 0.2 eV and 0.3 eV for Al and Ti [20], respectively, and N_D of 1×10^{15} cm^{-3} for both types of the substrate. Since $\phi_{bn,0}$ (or $\phi_{bp,0}$) is strongly influenced by β, an understanding of β is thus important for both the Schottky and ohmic contacts. The β data extracted from different Schottky-barrier diodes are listed in Figs. 5(a) and 5(b) for the Al and Ti contacts, respectively. Note that although different values of $\phi_{bn,0}, C_i, D_{it,0}, \phi_m - \chi$, and E_1 have been obtained and used, the values for β are still accumulated between 0.35 and 0.42 for the Al and Ti contacts on both types of the substrate.

In the past, $\beta = q\phi_0/E_g$ has been recognized as a property of a semiconductor and was assumed to be independent of the metal [9]. Although the values for β in our experiments are located within a limited range, it is identified mainly due to the fact that these diodes have all received the same surface treatments, e.g., dipping in the diluted HF solution and depositing the metal film using the same evaporator under the similar vacuum. This fact also implies that β is a strongly process-dependent parameter and can be used to predict the dependence of $\phi_{bn,0}$ (or $\phi_{bp,0}$) on a specified process. Therefore, by analyzing the characterization constant β, a particular process can be evaluated and its effects on the ohmic contacts can be further predicted.

Since the Schottky-barrier diodes and the ohmic contacts are simultaneously processed, it is now interesting to study the dependence of the ohmic contacts on the interface parameters deduced from the characteristics of the Schottky-barrier diodes. Figs. 7(a) and 7(b) show typical plots of the contact resistance vs the contact area for the Al and Ti contacts on both types of the heavily-doped substrate, respectively. In general, the measured data are concentrated around the line with a slope of -1. This fact indicates that the parasitic current crowding effects [21] have been minimized by using the self-aligned CBKR. The heavily doped p^+/n and n^+/p junctions are measured, and the results are shown in Fig. 8. The junction depth and the surface doping concentration are $0.2\,\mu$m and 4×10^{19} cm^{-3} for the p^+/n junction and $0.3\,\mu$m and 1×10^{19} cm^{-3} for the n^+/p junction, respectively.

Using the extracted interface parameters listed in Figs. 4 and 5 and considering N_S and m_t^* for both types of (100)-oriented Si-substrates [22], the theoretical curves for ρ_c versus N_S can be calculated, as shown in Fig. 9 for the Al and Ti contacts, respectively. For comparison, the curves considering the effects of the impurity band and the parabolic band on ρ_c are plotted. Clearly, the measured ρ_c versus N_S data show more satisfactory agreements with the theoretical results including the impurity band. This fact indicates that the high-doping effects can not be neglected for a heavily doped substrate. Although there still exist some uncertainties in accurately determining N_S from the SRP measurement, it is shown that once the implantation damage can be fully eliminated by a thermal activation process, the strongly process-dependent characterization parameter, e.g., $\phi_{bn,0}$ (or $\phi_{bp,0}$), should be carefully predetermined in order to clearly analyze the measured ρ_c data. Moreover, only when $\phi_{bn,0}$ (or $\phi_{bp,0}$) is first unambiguously determined, other effects which can result in the variations of ρ_c, e.g., the modification of N_S due to the dry-etching process, the metal-

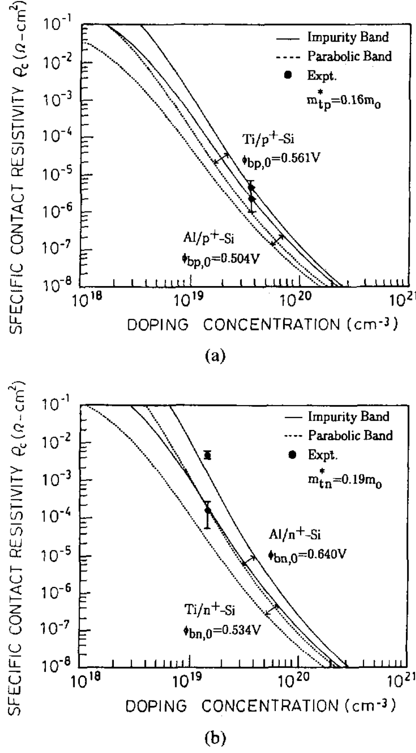


Fig. 9. The calculated and measured ρ_c versus N_S for Al/Si and Ti/Si ohmic contacts on (a) p-type and (b) n-type substrates.

silicon interaction, or the thermal silicidation [15], can be included and can be separately discussed without confusion.

IV. Conclusions

A self-consistent interfacial-layer model and a characterization method have been developed to study the effects of the interface properties on both the nonideal current transport behavior of the Schottky-barrier diodes and the degradation characteristics of the ohmic contacts. It has been shown that the thermal-equilibrium barrier height, which is an important parameter for determining the ohmic contacts, is very sensitive to process-related factors, e.g., the interfacial-layer capacitance, and the dominant type of interface states and their density distributions within the energy bandgap. Moreover, the specific contact resistivity ρ_c has been found to become less dependent on the type of the substrate and the kind of metal as the density of the interface states increases beyond a certain critical value. Experiments have been performed to extract the physical parameters of the interface states from the Schottky-barrior diodes as well as the nearly true specific contact resistivity from a self-aligned cross bridge Kelvin resistor. It has been shown that the characteristics of the thermal-equilibrium barrier height and the ohmic contacts can be consistently interpreted in terms of the interface properties. Therefore, the quality of the ohmic contacts can be diagnosed by analyzing the interface parameters deduced from the simultaneously processed Schottky-barrier diodes even though their behavior deviates from ideality.

Appendix

As the impurity concentration in the semiconductor increases, the splitting of the impurity energy level into a band occurs due to the interactions between the introduced impurity atoms themselves. The density of states for the impurity band can be expressed as [23]

$$D_i(E) = 2N_S(2\pi\delta^2)^{-1/2}\exp\left(-\frac{(E-E_D)^2}{2\delta^2}\right) \quad \text{(A1)}$$

where E_D is the donor energy level, and δ is the standard deviation of the impurity band given by

$$\delta = q^2\left(\frac{\lambda N_S}{8\pi\epsilon_s^2}\right)^{1/2} \quad \text{(A2)}$$

in which λ is the screening length of the Coulomb potential, which can be expressed as

$$\lambda = \left[\frac{2q}{\hbar}\left(\frac{3}{\pi}N_S\right)^{1/6}\left(\frac{m_d^*}{4\pi\epsilon_s}\right)^{1/2}\right]^{-1}. \quad \text{(A3)}$$

The periodic potential of the host lattice is strongly disturbed by the interactions between host atoms and impurity atoms. As a result, the conduction band is tailing off gradually into the bandgap. The modified density of states for the conduction band can be expressed as [24]

$$D_c(E) = \frac{m_d^*(2^{3/2}\delta)^{1/2}}{\pi^2\hbar^3}y\left(\frac{E}{\sqrt{2}\delta}\right) \quad \text{(A4)}$$

where δ is shown in (A2), and $y(x)$ can be expressed as

$$y(x) = \sqrt{\pi}^{-1}\int_{-\infty}^{x}(x-\zeta)^{1/2}\exp(-\zeta^2)d\zeta. \quad \text{(A5)}$$

Considering these high-doping effects, the effective density of states $D(E)$ can be given by the envelope of $D_i(E)$ and $D_c(E)$:

$$D(E) = \max[D_i(E), D_c(E)]. \quad \text{(A6)}$$

Since the density of states found in an incremental energy range $D(E)dE$ is equal to $2(1/2\pi)^3 dk_x dk_y dk_z$ within an incremental volume in k space, therefore, (10) can be rewritten as [16]

$$J_t = \iiint qv_x[F_s(E) - F_m(E)]T_t(E_x)2\left(\frac{1}{2\pi}\right)^3 dk_x dk_y dk_z. \quad \text{(A7)}$$

For a spherical energy surface and with an isotropic density-of-state mass m_d^*, (A7) can be simplified as

$$J_t = \frac{A^*}{k_b^2}\int_{E_c'}^{E_c'+qV_b}\int_0^{\infty}[F_s(E) - F_m(E)]T_t(E_x)dE_\perp dE_x \quad \text{(A8)}$$

in which A^* is the effective Richardson constant; k_b is the Boltzmann constant; and $E_x = \hbar k_x^2/2m_d^*$ and $E_\perp = \hbar k_y^2/2m_d^* + \hbar k_z^2/2m_d^*$. Under the conservation of the total momentum, the relationship between E and $E_x + E_\perp$ for a heavily-doped semiconductor can be obtained using the following method.

Since the total number of states n is assumed to be confined within a sphere in k space and the integration of $D(E)$ over the electron energy can also yield an expression for n, therefore, we obtain:

$$k(E) = \left[3\pi^2 \int_{-\infty}^{E} D(E)dE\right]^{1/3}. \qquad (A9)$$

Equation (A9) indicates that the effective energy-momentum relation can be obtained from the predetermined $D(E)$, and thus the dependence of $E_x + E_\perp$ on E can be obtained. Note that only at low doping concentrations, E will be equal to $E_x + E_\perp$ as conventionally used for a parabolic band.

References

[1] Y. El-Mausy, "MOS device and technology constraints in VLSI," *IEEE Trans. Electron Devices,* vol. ED-29, pp. 567–573, 1982.

[2] K. K. Ng and W. T. Lynch, "The impact of intrinsic series resistance on MOSFET scaling," *IEEE Trans. Electron Devices,* vol. 34, pp. 503–511, 1987.

[3] F. A. Padovani and R. Stratton, "Field and thermionic-field emission in Schottky barriers," *Solid-State Electron,* vol. 9, pp. 695–707, 1966.

[4] A. Y. C. Yu, "Electron tunneling and contact resistance of metal-semiconductor barrier," *Solid-State Electron.,* vol. 13, pp. 239–247, 1970.

[5] C. Y. Chang, Y. K. Fang, and S. M. Sze, "Specific contact resistance of metal-semiconductor barrier," *Solid-State Electron.,* vol. 14, pp. 541–550, 1971.

[6] P. Muret and A. Deneuville, "Capacitance spectroscopy of localized states at metal semiconductor interfaces I. theory," *J. Appl. Phys.,* vol. 53, pp. 6291–6299, 1982.

[7] P. Muret, "Capacitance spectroscopy of localized states at metal semiconductor interfaces II. experiments about Ag, Au, and Ni on crystalline (111) Si surfaces," *J. Appl. Phys.,* vol. 53, pp. 6300–6307, 1982.

[8] H. H. Tseng and C. Y. Wu, "A simple technique for measuring the interface-state density of the Schottky barrier diodes using the current-voltage characteristics," *J. Appl. Phys.,* vol. 61, pp. 299–304, 1987.

[9] A. M. Cowley and S. M. Sze, "Surface states and barrier height of metal-semiconductor systems," *J. Appl. Phys.,* vol. 36, pp. 3212–3220, 1965.

[10] C. Y. Wu, "Interfacial layer-thermionic-diffusion theory for the Schottky barrier diodes," *J. Appl. Phys.,* vol. 53, pp. 5847–5950, 1982.

[11] E. H. Nicollian and A. Goetzberger, "The Si-SiO_2 interface electrical properties as determined by the metal-insulator-silicon conductance technique," *Bell Sys. Tech. J.,* vol. 46, pp. 1055–1133, 1967.

[12] P. V. Gray and D. M. Brown, "Density of Si-SiO_2 interface states," *Appl. Phys. Lett.,* vol. 8, pp. 31–33, 1966.

[13] D. M. Brown and P. V. Gray, "Si-SiO_2 fast interface state measurement," *J. Electrochem. Soc.,* vol. 115, pp. 760–766, 1968.

[14] S. M. Sze and J. C. Irvin, "Resistivity, mobility and impurity levels in GaAs, Ge, and Si at 300°K," *Solid-State Electron.,* vol. 11, pp. 599–602, 1968.

[15] Y. S. Lou and C. Y. Wu, "A characterization technique for the degradation characteristics of Ti/Si Schottky barrier diodes and ohmic contacts after thermal silicidation," *Solid-State Electronics,* to be published.

[16] J. W. Conley, C. B. Duke, G. D. Mahan, and J. J. Tiemann, "Electron tunneling in metal-semiconductor barriers," *Phys. Rev.,* vol. 150, pp. 466–469, 1966.

[17] P. Cappelletti, M. Finetti, A. Scorzoni, I. Suni, N. Circelli, and G. Dalla Libera, "Current crowding and misalignment effects as sources of error in contact resistivity measurements: part II-experimental results and computer simulation of self-aligned test structure," *IEEE Trans. Electron Devices,* vol. 34, pp. 532–536, 1987.

[18] J. H. Werner and H. H. Guttler, "Barrier inhomogeneities at Schottky contacts," *J. Appl. Phys.,* vol. 69, pp. 1522–1533, 1991.

[19] R. T. Tung, "Electron transport at metal-semiconductor interfaces: general theory," *Phys. Rev. B,* vol. 45, pp. 509–523, 1992.

[20] H. B. Michaelson, "Relation between an atomic electronegativity scale and the work function," *IBM J. Res. Dev.,* vol. 22, pp. 72–80, 1978.

[21] W. M. Loh, S. E. Swirhun, T. A. Schreyer, R. M. Swason, and K. C. Saraswat, "Modeling and measurement of contact resistances," *IEEE Trans. Electron Devices,* vol. 34, pp. 512–524, 1987.

[22] K. K. Ng and R. Liu, "On the calculation of the specific contact resistivity on (100) Si," *IEEE Trans. Electron Devices,* vol. 37, pp. 1535–1537, 1990.

[23] T. N. Morgan, "Broadening of impurity bands in heavily doped semiconductor," *Phys. Rev.,* vol. 139, pp. 343–348, 1965.

[24] E. O. Kane, "Thomas Fermi approach to impure semiconductor band structure," *Phys. Rev.,* vol. 131, pp. 79–88, 1963.

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