Specific contact resistivity of n-type Si and Ge M-S and M-I-S contacts

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Abstract—We have theoretically investigated the specific contact resistivity of n-type Si and Ge metal-insulator-semiconductor contacts with various insulating oxides. We have found a significant reduction of the contact resistivity for both Si and Ge with an insertion of insulators at low and moderate donor doping levels. However, at the higher doping levels (>10^{19} cm^{-3}), the reduction of the contact resistivity is negligible and the contact resistivity increases as the insulator thickness increases. Thus, we have shown that the lowest possible contact resistivity can be achieved with the metal-semiconductor contact with highest possible activated doping density.

I. INTRODUCTION

As the semiconductor devices scale down to nanometer regime, the contact resistance becomes dominant component of parasitic resistance of the devices. Thus, it is urgently required to reduce the contact resistance to meet the performance target of the future 7nm and beyond technology nodes. According to the ITRS roadmap [1], the maximum specific contact resistivity $\rho_c$ is required to be 1.5 x 10^{-9} Ω.cm² by 2028 to meet the overall parasitic resistance requirement in the silicon (Si) MOSFET devices. In a theoretical study on the intrinsic limit of the contact resistivity within the ballistic transport limit, it has been shown that the ITRS target is indeed possible from a theoretical perspective in a moderate doping density range for Si [2]. Yet, the lowest specific contact resistivity reported in an experiment so far for the p-type metal-semiconductor (M-S) contact (Pt-Si) is $\rho_c = 1.9 x 10^{-9}$ Ω.cm² [3]. In order to further reduce the contact resistivity, metal-insulator-semiconductor (M-I-S) contacts have been proposed and demonstrated to depin the metal Fermi-level by inserting an ultrathin insulating layer in between metal and semiconductor leading to a reduced Schottky barrier height so the lower the contact resistivity [4]–[7]. The Schottky barrier height reduction by the Fermi level depinning effect has been theoretically investigated within the metal induced gap states (MIGS) theory [8]–[10] which has been extensively adopted in the M-I-S contact resistivity modeling to seek an optimized insulator thickness for the lowest possible contact resistivity [11], [12].

In this study, we have employed MIGS modeling [13] to describe the Fermi-level depinning due to an ultrathin insulator in between the metal and semiconductor layers. We also have employed a tunneling model based on the transfer matrix method (TMM) to calculate the tunneling current across the given potential barrier profile. Then we have evaluated the contact resistivity as a function of doping density and insulator layer thickness for a given M-I-S contact.

II. METHODOLOGY

Figure 1 (a) shows the schematic band diagram of the Schottky barrier for the M-S contact where the metal workfunction, electron affinity, charge neutrality level, Schottky barrier height, Fermi level, vacuum level, conduction and valence band edge of the semiconductor are denoted as $\Phi_m$, $\chi_s$, $\phi_{CNL}$, $\phi_n$, $E_{FS}$($E_{FS}$), $E_{vac}$, $E_c$, and $E_v$, respectively.

$$V(z) = \frac{q^2 N_D}{2\epsilon_s} (W_D - z)^2 - \frac{q^2}{16\pi\epsilon_s^2} z,$$  

(1)

where the $N_D$ is the doping density in the semiconductor, permittivity of the semiconductor $\epsilon_s=11.7\epsilon_0$, and the depletion width $W_D = \sqrt{2\epsilon_s(V_{ba} - V) / qN_D}$. $V$ is the applied bias voltage to the contact and the surface potential is $qV_{ba} = \phi_n - (E_c - E_{FS})$ where the position of the conduction band relative to the Fermi-level is approximated as [15],

$$\frac{E_c - E_{FS}}{k_BT} = \left(\frac{3\sqrt{\pi\gamma}}{4}\right)^{2/3} + \frac{8\sqrt{\pi\gamma}}{3(4 + \sqrt{\pi\gamma})^2},$$  

(2)

where $k_BT$=0.0258 eV at $T=300$ K and the $\gamma = N_D/N_c$. The effective density of states for electrons is $N_c = 2/(2\pi m_e^*k_BT/h^2)^{3/2}$ where $m_e^*$ is the electron effective mass and $N_D$ and $N_c$ are the doping density and effective density of states for electrons, respectively. Note that the metal Fermi-level $E_{FS}$ is aligned to the charge neutrality level ($\phi_{CNL}$) (measured from the valence
band maximum) of the Si due to the MIGS density near the interface leading to the Fermi-level pinning. Thus the Schottky barrier height is determined by the Fermi-level pinning factor $S$ [10], [16] and the $\Phi_S$ which is measured from the vacuum to the $\phi_{CNLS}$,

$$\phi_n = S(\Phi_m - \Phi_S) + (\Phi_S - \chi_s) .$$  (3)

The pinning factor $S$ is related to the MIGS density as following [17],

$$S = \frac{1}{1 + (q^2D_{MIGS,0}\delta_s)/(\epsilon_s)} ,$$  (4)

where the $D_{MIGS,0} = 1/(\pi\alpha^2E_b)$ is the MIGS density at zero insulator thickness in between the metal and semiconductor contact. $\alpha$ is the atomic bonding length, $\delta_s$ is the MIGS decay length [9] and the $E_b$ is the band gap of the semiconductor. We have used material parameters for semiconductors and metal workfunctions as shown in Table I and II and the calculated pinning factor $S$ is shown in Table I.

With an insertion of an insulator layer in between the metal and semiconductor contact as shown in Fig. 1 (b), we can re-write the Eq. 3 as,

$$\phi_n = \Phi_S - \chi_s - \psi_s ,$$  (5)

where the equilibrium surface potential corresponding to the total band bending within the semiconductor [13],

$$\psi_s(C_s) = -\frac{C_I}{C_I + C_S}\Phi_{MS} - \frac{C_I}{C_I + C_{IS}}\Delta_{IS} ,$$  (6)

where the $C_I$ and $C_S$ are the surface capacitance densities for the insulator and semiconductor, respectively, while $C_{IS}$ are insulator-semiconductor dipole capacitance densities for the insulator and semiconductor, respectively. $\Delta_{IS}$ is the insulator-semiconductor dipole voltage,

$$\Delta_{IS} = (1 - S_{IS})[\phi_{CNLS} - \phi_{CNLI}] ,$$  (7)

where the $S_{IS}$ is the pinning factor for the insulator-semiconductor interface and the $\phi_{CNLS}$ is the charge neutrality level of the insulator as listed in Table III for various insulators. In order to evaluate the n-type SBH in Eq. 5, the surface potential $\psi_s$ should be assessed simultaneously which is described in more detail in Refs. [12], [13], [18]. Note the $\Phi_{MS}$ in Eq. 6 is,

$$\Phi_{MS} = \Phi_{M,eff} - \Phi_S ,$$  (8)

where the effective metal workfunction $\Phi_{M,eff}$ is given as,

$$\Phi_{M,eff} = S(t_{ox})\Phi_M + [1 - S(t_{ox})]S(t_{ox})\Phi_S ,$$  (9)

in terms of the insulator thickness dependent pinning factor,

$$S(t_{ox}) = \left(1 + q^2D_{MIGS}(t_{ox})(\delta_{s0}\epsilon_{ox} + t_{ox}\epsilon_s)\right)^{-1} ,$$  (10)

where the $t_{ox}$ is the insulator thickness and $\epsilon_{ox}$ is the dielectric constant of the insulator. Also, the insulator thickness dependent MIGS density can be written as,

$$D_{MIGS}(t_{ox}) = D_{MIGS,0}\exp[-t_{ox}/\delta_{ox}] ,$$  (11)

where $\delta_{ox} = 2h^2\pi/(\mu_{e0}\alpha_{ox}E_{F,ox})$ where the $\alpha_{ox}$ and $E_{F,ox}$ are the lattice constant and band gap of the insulator, respectively [17]. Note the Eqs. 5, 10 and 11 consistently converge to the Eqs. 3 and 4 without the insulator layer (i.e. $t_{ox} \rightarrow 0$).

Once we have established 1D homogeneous Schottky barrier profile with and without an insulator layer using the MIGS theory, we then have calculated the net current density using the Tsu-Esaki formula within parabolic band and effective mass approximation [19],

$$J = \sum_{i=1}^{nvalley} m_{i,e}^*k_BT \int_{E_{min}}^{\infty} dE_zT_z(E_z)\ln \left\{1 + \frac{1 + e(E_{FM} - E_z)/k_BT}{1 + e(E_{FM} - E_z)/k_BT} \right\} ,$$  (12)

where $m_{i,e}^*$ is the orientation dependent conductivity effective mass at each equi-energy surface (represented by index $i$ and the number of equi-energy surface ‘nvalley’ is six and four at the conduction band minimum of Si and Ge, respectively ) [20]. We have taken into account the multi-valley tunneling by summing up the current density at all conduction band valleys. The tunneling probability $T_z(E_z)$ at a given incident electron energy $E_z$ at each conduction band valley $i$ is evaluated using the conventional transfer matrix method (TMM) [21] with a boundary condition used in Ref. [22],

$$T_z(E_z) = \frac{m_{i,e}^*_{tun,N+1}k_{N+1}k_0}{m_{i,e}^*_{tun,0}k_0k_{N+1}} \left[\frac{k_0}{k_{N+1}}\right]^2 \left[\frac{1}{M_{22}}\right] ,$$  (13)

where the indices 0 and $N + 1$ represent the first (in the metal) and last (in the semiconductor) discretized grid points across the potential barrier profile, $M_{22}$ is the matrix element of the transfer matrix and the wavevector $k_{N+1} = \sqrt{2m_{i,e}^*_{tun,N+1}(E_z - V_{N+1})}/\hbar$. Note that we have used the orientation dependent tunneling effective mass $m_{i,e}^*_{tun}$ at each conduction band valley $i$ [23] when evaluating the tunneling probability. Finally, the specific contact resistivity $\rho_c = dV/dI$ is then numerically evaluated at a very small applied voltage $V = 10^{-5}$ V at which the $\rho_c$ converges by varying $V$.

### III. RESULTS AND DISCUSSIONS

Figure 2 (a) shows the $\rho_c$ for the n-type M-S contact for (001) Si at a given Schottky barrier height varying from 0.2 eV to 0.8 eV as a function of donor doping density at $T=300$ K. As expected the $\rho_c$ is smaller at lower barrier height and continuously decreases as the doping density increases. In addition, the barrier height dependence on the $\rho_c$ becomes

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### Table I. Material parameters for semiconductors

<table>
<thead>
<tr>
<th>Material</th>
<th>$E_g$ (eV)</th>
<th>$\epsilon_{\infty}$</th>
<th>$S$</th>
<th>$\chi$ (eV)</th>
<th>$\phi_{CNLS}$ (eV)</th>
<th>$\alpha$ (Å)</th>
<th>$\delta_s$ (Å)</th>
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### Table II. Metal workfunctions

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<td>Al</td>
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<td>Au</td>
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### Table III. Material parameters for insulators

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<th>$E_g$ (eV)</th>
<th>$\chi$ (eV)</th>
<th>$\phi_{CNLS}$ (eV)</th>
<th>$a_0$ (Å)</th>
<th>$m^*$ (m_0)</th>
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<td>6.0</td>
<td>2.0</td>
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<tr>
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<td>3.25</td>
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negligible at ultra high doping region (\(N_d > 10^{21} \text{ cm}^{-3}\)) and the \(\rho_c\) converges to \(2.1 \times 10^{-9}\) and begins to increase with even higher doping which is due to the interplay between the matrix element \(M_{22}\) and the wavevector \(k_{N+1}\). Because the wavevector \(k_{N+1}\) in Eq. 13 becomes dominant at very high dopings as the Fermi-level deeply penetrates into the conduction bands while the matrix element \(M_{22}\) converges to unity. Thus the tunneling probability is reduced which leads to the decreased tunneling current.

Figure 2 (b) shows that there is only slight differences in \(\rho_c\) between Si and Ge at a given barrier height and at a given crystal orientation. Also, a slight orientation dependence can be seen in Fig. 2 (c) (lower \(\rho_c\) with (001) orientation for Si while lower

\[\rho_c \approx 4.02 \times 10^{-6} \text{ cm}^{-1}\] for Ge

\[\rho_c \approx 3.04 \times 10^{-6} \text{ cm}^{-1}\] for Si

Having discussed the \(\rho_c\) for the M-S contact, we have shown the \(\rho_c\) as a function of insulator thickness (\(t_{ox}\)) for M-I-S contact in Fig. 3 with various insulators (\(\text{HfO}_2\), \(\text{La}_2\text{O}_3\), \(\text{Al}_2\text{O}_3\), \(\text{TiO}_2\), \(\text{Si}_3\text{N}_4\), \(\text{GeO}_2\), \(\text{ZnO}\)) for Si and Ge with Ti as a contact metal. As clearly seen in Fig. 3 (a) and (c), the \(\rho_c\) can be significantly reduced (up to two orders of magnitude) by an insertion of insulating layers for both Si and Ge at moderate doping level \(N_d=10^{20} \text{ cm}^{-3}\) due to the Fermi-level depinning effect leading to reduced Schottky barrier height \([7], [12], [18]\). However, the \(\rho_c\) begins to increase when the thickness of the insulator becomes thicker than their optimized thicknesses as the barrier tunneling through the insulator offsets the \(\rho_c\) benefit from the reduced barrier height. We have found that the lowest \(\rho_c\) can be achieved with \(\text{Si}_3\text{N}_4\) for Si and \(\text{ZnO}\) for Ge with optimized insulator thicknesses of \(t_{ox} \sim 0.5 \text{ nm}\) and \(t_{ox} \sim 3.0 \text{ nm}\), respectively, at the moderate doping density. However, there is no (or negligible) reduction of the \(\rho_c\) by the insulator at high doping density \(N_d=10^{20} \text{ cm}^{-3}\) as shown in Fig. 3 (b) and (d) because the \(\rho_c\) benefit from the reduced
barrier height becomes negligible at high doping density as already shown in Fig. 2. It is worth to note that the $\rho_c$ at the high doping $N_D=10^{20} \text{cm}^{-3}$ without the insulator (i.e., M-S contact) is still lower than the $\rho_c$ at the moderate doping $N_D=10^{19} \text{cm}^{-3}$ with optimized insulator thickness. Therefore we can conclude that there is no benefit (or at least questionable benefit) for the lowest possible $\rho_c$ by employing the M-I-S contact with ultra high doping density.

One can see more clearly in Fig. 4 that the lowest $\rho_c$ for both Si and Ge can be achieved at $N_D=10^{20}$ (or higher doping density) with M-S contact as opposed to the previous theoretical calculations \cite{12, 18}. The same trend has been also confirmed by our experiment on the contact resistance of Ti/TiO$_2$ (1nm)/Si contact as shown in Fig. 5 (b) in which slightly lower contact resistance was observed from the M-S contact at higher doping level $N_D=4\times10^{20} \text{cm}^{-3}$. However, the improvement (or degradation) of the resistance at high (or lower) doping level is not so significant as the calculated $\rho_c$ as shown in Fig. 5 (a) in which the $\rho_c$ improvement (or degradation) is about 10 times (or 100 times) at high (or lower) doping density from the M-S contact when compared the M-I-S contact. We believe that the small improvement of the resistance from the experiment at high doping is due to the existence of the native oxides as well as the poor quality of the interface formation.

IV. CONCLUSION

We have theoretically calculated the contact resistivity for M-S and M-I-S contacts with various insulators. We have employed MIGS modeling to describe the Fermi-level depinning effect by an insertion of the insulator in between the metal and semiconductor contact. Also, we have calculated the current density across the Schottky barrier profile within the parabolic and effective mass approximation by considering multi-valley and orientation dependent effective masses. We have shown that it is critically required to maximize the activated doping density in the M-S contact to achieve the lowest possible contact resistivity regardless of the crystal orientation, metal and semiconductor. In addition, we have also shown that the lowest contact resistivity can be achieved with M-S contact with ultra high doping density rather than M-I-S which is consistently observed from our experiment on contact resistance in Ti/TiO$_2$/Si contact.

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