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Contact resistivities of metal-insulator-semiconductor contacts and metal-semiconductor contacts

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Applying simulations and experiments, this paper systematically compares contact resistivities ($\rho_c$) of metal-insulator-semiconductor (MIS) contacts and metal-semiconductor (MS) contacts with various semiconductor doping concentrations ($N_d$). Compared with the MS contacts, the MIS contacts with the low Schottky barrier height are more beneficial for $\rho_c$ on semiconductors with low $N_d$, but this benefit diminishes gradually when $N_d$ increases. With high $N_d$, we find that even an “ideal” MIS contact with optimized parameters cannot outperform the MS contact. As a result, the MIS contacts mainly apply to devices that use relatively low doped semiconductors, while we need to focus on the MS contacts to meet the sub-10^{-8} $\Omega$ cm^{2} $\rho_c$ requirement for future Complementary Metal-Oxide-Semiconductor (CMOS) technology. Published by AIP Publishing.

Similar to Yu,36 we focus on semiconductors with $N_d$ of 10^{18}–10^{21} cm^{-3}, whose carrier conduction through the contact is based on thermionic-field emission (TFE) or field emission (FE).35 Carrier tunneling is the underlying mechanism behind TFE and FE; hence, the carrier tunneling probability, $P$, is the key variable in the $\rho_c$ calculation. Assuming parabolic energy-momentum relations in the semiconductor, the WKB approximations simplify the $P$ calculation to

$$\ln P(E_x) = -x \int_0^w [\phi(x) - E_x]^{1/2} dx,$$

(1a)

$$E_x = \frac{p_x^2}{2m},$$

(1b)

$$x = \frac{2(2m^*)^{1/2}}{\hbar},$$

(1c)

where $\phi(x)$ is the potential energy equation that describes the shape of the barrier, $w$ is the barrier width, $E_x$ and $p_x$ are the carrier energy and the carrier momentum perpendicular to the barrier, $m^*$ is the effective carrier mass, and $\hbar$ is the reduced Planck’s constant. Since (1a) cannot be solved analytically for an arbitrary $\phi(x)$ equation, Stratton applies the Taylor expansion to it

$$\ln P(E_x) = -(b + c\epsilon_x + f\epsilon_x^2 + ...),$$

(2a)

$$\epsilon_x = E_x - E_x,$$

(2b)

$$b = x \int_0^w [\phi(x) - E_x]^{1/2} dx,$$

(2c)

$$c = \frac{1}{2} x \int_0^w [\phi(x) - E_x]^{-1/2} dx,$$

(2d)

$$f = \frac{1}{8} x \int_0^w [\phi(x) - E_x]^{-3/2} dx,$$

(2e)
where $\epsilon_s$ is an intermediate variable that transforms (1a) into an equation with respect to the reference energy level, $E_r$. In other words, (2a) is a Taylor series of (1a) at the energy level $E_r$. The quadratic and higher order terms in (2a) can be neglected if the boundary condition $1 - c kT > k T \sqrt{2 q E}$ is met.\textsuperscript{35} In principle, $E_r$ should be selected close to the level where there is a maximum carrier tunneling.\textsuperscript{34}

Applying Taylor series for the $\ln P(E_x)$ expression is remarkable: it not only enables a numerical calculation of tunneling probability for an arbitrary barrier but also simplifies the expression of the IV behavior. By placing the Schottky barrier equation, $\phi_b(x)$, into (2a), the IV behavior and $\rho_c$ for the MS contacts are successfully derived.\textsuperscript{35,36} Interestingly, we find that the influence of an insulator in MIS can also be incorporated into (1a) and (2a) in a simple way: the total tunneling probability $P(E_x)$ through MIS can be calculated by

$$P(E_x) = P_s(E_x) \times P_t(E_x), \quad (3)$$

i.e.,

$$\ln P(E_x) = \ln P_s(E_x) + \ln P_t(E_x), \quad (4)$$

where $P_s(E_x)$ and $P_t(E_x)$ are the tunneling probabilities through the semiconductor barrier and insulator barrier, respectively. Similar to (2a), we carry out the Taylor expansion for $\ln P_s(E_x)$ and $\ln P_t(E_x)$

$$\ln P_s(E_x) = -\int_0^w [\phi_s(x) - E_x]^{1/2} dx = -(\beta s + c s \epsilon_s + f s \epsilon_s^2, \ldots), \quad (5)$$

$$\ln P_t(E_x) = -\int_0^w [\phi_t(x) - E_x]^{1/2} dx = -(\beta t + c t \epsilon_t + f t \epsilon_t^2, \ldots), \quad (6)$$

where $\phi_s(x)$ are the potential barrier equations for the insulator, and $t$ is the insulator thickness. After calculating the Taylor series for $\ln P_s(E_x)$ and $\ln P_t(E_x)$ with (5) and (6), $\ln P(E_x)$ is easily calculated. Eventually, the $\rho_c$ of the MIS contacts is derived.\textsuperscript{36}

Following the aforementioned methodology, three steps are taken for the MIS $\rho_c$ calculations: (a) build the barrier equations $\phi_s(x)$ and $\phi_t(x)$; (b) derive the Taylor series for $\ln P_s(E_x)$ and $\ln P_t(E_x)$; and (c) calculate the $\rho_c$ of the MIS. As a case study, the MIS contacts on n-Si(100) are taken, and a schematic energy band diagram is shown in Fig. 1(a).

![Diagram](image)

FIG. 1. (a) Schematic band diagram of MIS on n-Si(100) including key parameters. With a constant $\phi_b$, MIS band diagram with (b) high $N_d$ and (c) intermediate $N_d$ is compared.

Similar to previous studies,\textsuperscript{35,36,38} we apply the 1D Poisson equation and the depletion approximation for $\phi_b(x)$

$$\phi_b(x) = \frac{qN_d}{2 \epsilon_r \epsilon_0} (w - x)^2, \quad (7a)$$

where

$$w = \sqrt{\frac{2 \epsilon_r \epsilon_0 (\phi_b - \epsilon_D)}{qN_d}}, \quad (7b)$$

$$\epsilon_D = E_C - E_F. \quad (7c)$$

$N_d$ is the active donor concentration, $w$ is the depletion width, $\epsilon_r$ is the relative dielectric constant of the semiconductor, $\epsilon_0$ is the vacuum electric permittivity, and $E_C$ and $E_F$ are the conduction band minimum and the Fermi energy level, respectively. The energy difference $\epsilon_D$ is a function of $N_d$, which is solved using the Fermi-Dirac distribution and dopant ionization functions.\textsuperscript{39,40}

To build $\phi_b(x)$, knowledge of the electric field in the insulator ($F_i$) is required. As a general discussion, we neglect the interfacial charges and the fixed charges in the insulator for simplicity. With continuity of the electric displacement, the electric field at the semiconductor surface ($F_{ss}$) and $F_i$ has the relation

$$\epsilon_{ss} F_{ss} = \epsilon_r \epsilon_0 F_i, \quad (8)$$

where $\epsilon_{ss}$ is the relative dielectric constant of the insulator. With the depletion approximation,

$$F_{ss} = \frac{qN_d w}{\epsilon_{ss} \epsilon_0}. \quad (9)$$

With (8),

$$F_i = \frac{qN_d w}{\epsilon_r \epsilon_0}. \quad (10)$$

Then,

$$\phi_b(x) = \phi_b + \Delta E_c - \epsilon_D - \frac{q^2 N_d w}{\epsilon_r \epsilon_0} x. \quad (11)$$

After building $\phi_b(x)$ and $\phi_b(x)$, we only need to define $E_R$ before carrying out the Taylor expansions. Since $E_R$ has to be defined close to the level that has a maximum carrier tunneling flux, different criteria have to be applied for FE and TFE, respectively. FE dominates when the semiconductor barrier is thin (Fig. 1(b)). In the previous works,\textsuperscript{34,36} $E_R$ is selected as $E_R$ for FE, because these studies cover the cryogenic operations: at cryogenic temperatures, the electrons close to $E_F$ have the highest kinetic energy and they also see the thinnest tunneling barrier. But at room temperature, $E_F$ is unfavorable as $E_R$, which makes those $\rho_c$ calculations\textsuperscript{35,36} invalid for low-$\phi_b$ contacts. Since this paper mainly focuses on $\rho_c$ at room temperature, considering the product of $D(E_x)$ and $P(E_x)$, we define $E_{R1} = E_F + 1.5 kT$ (k is the Boltzmann constant and T is the temperature) for FE, as shown in Fig. 1(b). This selection of $E_{R1}$ allows a more accurate and flexible $\rho_c$ calculation at room temperature, which also applies to low-$\phi_b$ contacts. Since at room temperature, FE is mainly related with degenerate...
semiconductors, whose $E_{R1}$ is located in the conduction band of the semiconductor, the range of the integral in (2a) needs to be modified from $0 \sim 0$ to $0 \sim w_1$. $w_1$ is the position near the semiconductor surface, where $E_c(w_1) = E_{R1}$. TFE dominates when the semiconductor barrier is relatively thick (Fig. 1(c)). In this case, most of the carrier tunneling occurs close to the top of $\phi_E(x)$ where the barrier is thin enough for carriers to tunnel through. For TFE, same as Stratton and Padovani, $E_{RM}$ is numerically calculated following the criterion $c_m kT = 1$ and (2d), where $c_m$ is the coefficient of the quadratic term in the Taylor series of $\ln(P(E_x))$ for FE. The above equation is valid when $(\sqrt{2a} + c_1)kT < 1$ and $\epsilon_D < 0$.

For TFE, $\rho_c$ is the Richardson constant, $m^*_c$ is the electron effective mass in the conduction band of the semiconductor, and $b_1$, $c_1$, and $f_1$ are the polynomial coefficients in the Taylor series of In $P(E_x)$ for FE. The above equation is valid when $(\sqrt{2a} + c_1)kT < 1$ and $\epsilon_D < 0$.

The $\rho_c$-Nd data of Ti/TiO$_2$/n-Si MS and Ti/TiO$_2$/n-Si MIS contacts and curve fitting. Each symbol is an averaged $\rho_c$ measured with four sets of CTLM or MR-CTLM. Dashed lines are fitting curves. The fitting parameter for Ti/n-Si is $\phi_B = 0.53\,eV$; and those for Ti/TiO$_2$/n-Si are $\phi_B = 1.0\,eV$, $t = 1.4\,nm$, $\Delta E_{EC} = 0.55\,eV$, $m^*_c = 0.3\,m_0$, and $\epsilon_i = 80$. The inset is an XTEM image of Ti/TiO$_2$/n-Si.

Interesting contrasts are observed in Fig. 2: for relatively low doped n-Si with $N_d < 2.0 \times 10^{18}$ and $1.5 \times 10^{19}$ cm$^{-3}$, the $\rho_c$ of Ti/TiO$_2$/n-Si is lower than that of Ti/n-Si; however, when $N_d$ is higher than $4 \times 10^{19}$ cm$^{-3}$, the Ti/n-Si outperforms the Ti/TiO$_2$/n-Si. The experimental data are then fitted using the $\rho_c$ model. Good agreements are achieved between the extracted $\phi_B$ from the fitting (Fig. 2) and $\phi_B$ from our previous Schottky barrier study where $\phi_B$ of Ti/n-Si is 0.46–0.48 eV, while $\phi_B$ of Ti/(~0.8 nm)TiO$_2$/n-Si is ~0.14 eV. Combined with the schematic of Figs. 1(b) and 1(c), the crossover of the $\rho_c$-Nd curves of Ti/n-Si and Ti/TiO$_2$/n-Si in Fig. 2 can be understood qualitatively: on lowly doped Si ($N_d < 4 \times 10^{19}$ cm$^{-3}$), the semiconductor barrier is thick and dominant, so that the thermionic-field emission (TFE) through Ti/TiO$_2$/n-Si with a low $\phi_B$ is much easier than that through Ti/n-Si; however, on highly doped Si, the semiconductor barrier becomes thin and minor compared with the TiO$_2$ barrier so that the field emission (FE) in Ti/n-Si is much easier than Ti/TiO$_2$/n-Si in spite of a relatively high $\phi_B$ of ~0.5 eV.

In the $\rho_c$-N$_d$ curve fitting for Ti/TiO$_2$/n-Si in Fig. 2, the TiO$_2$ thickness ($t$) is determined with XTEM, and the effective electron tunneling mass ($m^*_c$) and the dielectric constant ($\epsilon_i$) of TiO$_2$ are taken from the literature. The Ti/Si conduction band offset $\Delta E_C$ of ~0.55 eV and $\phi_B$ of ~0.1 eV are directly extracted from the fitting. The $\Delta E_C$ of ~0.55 eV is close to the values of 0.6–0.8 eV determined from the internal electron photoemission (IPE) spectroscopy and is different from the zero $\Delta E_C$ in the previous simulation reports. This is because the crystalline TiO$_2$ parameters are used in the simulation but an amorphous ALD TiO$_2$ is applied in the IPE experiment and in this work. The amorphous TiO$_2$ has a ~1 eV larger band gap and a much higher $\Delta E_C$ with respect to Si than the crystalline TiO$_2$. In the previous MIS simulation studies, Roy et al. and Agrawal et al. concluded that TiO$_2$ is an optimal candidate for the MIS contacts on n-Ge or n-Si. These conclusions are actually based on the zero $\Delta E_C$ assumption of TiO$_2$, while the realistic $\Delta E_C$ of ~0.6 eV clearly makes amorphous TiO$_2$ a less ideal candidate for MIS. Unfortunately, the as deposited ~1 nm
ALD TiO$_2$ is always at an amorphous state, while we found that the thermal treatment at even 750°C can hardly crystallize this ultrathin TiO$_2$.

After the case study of the Ti/n-Si and Ti/TiO$_2$/n-Si contacts, it is interesting to generally compare the lower $\rho_c$ limits between the MS and MIS contacts. For MS contacts, $N_d$ and $\phi_b$ are dominating factors. As shown in Fig. 2, ultrahigh $N_d$ approaching $1 \times 10^{21}$ cm$^{-3}$ is achievable for n-Si.$^{4,41}$ With rare earth silicides as contact metal, low $\phi_b \sim 0.3$ eV have been demonstrated for MS contacts.$^{49,50}$ For MIS contacts, as shown in Fig. 3, their $\rho_c$ correlates strongly with $\phi_b$, $t$, $m^*_c$, and $\Delta E_C$. For instance, in Fig. 2, the relatively high $t$, $m^*_c$, and $\Delta E_C$ of the Ti/TiO$_2$/n-Si contacts lead to a high $\rho_c$ above $1 \times 10^{-6}$ $\Omega$·cm$^2$ even with $N_d$. In Fig. 4, we hypothetically model an “ideal” MIS with optimized parameters on n-Si (A) and compare it with the TiO$_2$ MIS reference in Fig. 2 (B) and the MS references with $\phi_b$ of 0.1 eV (C) and 0.3 eV (D). (Because of the Fermi-level pinning at the Si surface, $C$ does not exist in reality.)

In Fig. 4, we see that the $\rho_c$-$N_d$ curves of A, B, and C are almost in parallel, which means that the insulator in the MIS contacts augments $\rho_c$ by a similar degree for any $N_d$. The advantage of the MIS contacts is most pronounced at relatively low doping levels, but it diminishes gradually with increasing $N_d$—at ultrahigh doping levels, even the “ideal” MIS, A, cannot outperform its MS counterpart. D. Moreover, the existence of such an “ideal” MIS as A is suspicious: for instance, insulators with $m^*_c$ as low as 0.2 $m_0$ are uncommon;$^{46,50}$ insulators that have low $\Delta E_C$ with semiconductors are rare;$^{51,46,46,50}$ moreover, there is usually a minimal insulator thickness of $> 1$ nm required for an MIS to lower $\phi_b$ to 0.1 eV.$^{5,7,9,13}$ In conclusion, the MIS contacts are more appealing to the applications that use relatively low doped semiconductors, such as compound semiconductor devices and Si solar cells, while the MS contacts will still be the major force to push $\rho_c$ down below $1 \times 10^{-8}$ $\Omega$·cm$^2$ to meet the Complementary Metal-Oxide-Semiconductor (CMOS) requirement for the 10 nm technology node and beyond.$^{51}$

In summary, this paper systematically compares the contact resistivity of the MIS and MS contacts. A model is built for the quantitative $\rho_c$ study and is verified by experiments. We find that the MIS contacts are more preferable on relatively low doped semiconductors due to their efficient Schottky barrier height modulation. However, on highly doped semiconductors, whose contact resistivity is much less sensitive to Schottky barrier height, the MS contacts are more desirable because of their less carrier tunneling difficulty.

FIG. 3. Simulation of $\rho_c$-$N_d$ curves of MIS contacts using a set of default parameters: $\phi_b = 0.1$ eV, $t = 1$ nm, $\Delta E_C = 0.5$ eV, $m^*_c = 0.3 m_0$, and $\epsilon_0 = 80$. Then, based on default settings, (a) $\phi_b$, (b) $t$, (c) $\Delta E_C$, and (d) $m^*_c$ are varied individually to illustrate their impacts on $\rho_c$.

FIG. 4. Comparison of $\rho_c$-$N_d$ curves of MIS and MS on n-Si(100) based on simulations. The curves are named with A–D for simplicity. A is hypothetically assigned with superior parameters: $\phi_b = 0.1$ eV, $t = 0.5$ nm, $\Delta E_C = 0.1$ eV, and $m^*_c = 0.2 m_0$, B is the Ti/TiO$_2$/n-Si MIS fitting curve in Fig. 2 with parameters of $\phi_b = 0.1$ eV, $t = 1.4$ nm, $\Delta E_C = 0.55$ eV, and $m^*_c = 0.3 m_0$. C and D are MS references. The green and red arrows denote the $\rho_c$ differences between A and D.