Lower Limits To Specific Contact Resistivity

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***Abstract* — We calculate minimum feasible contact resistivities to n-type and p-type InAs and $In_{0.53}Ga_{0.47}As$. Resistivities were calculated for a range of Schottky barrier heights as well as for the case where the transmission probability is unity (Landauer limit). Calculations are compared with recent experimental data. Experimental contact resistivities for *n*-$In_{0.53}Ga_{0.47}As$ and *n*-InAs lie within 2.5:1 of calculated resistivities given generally accepted values of Schottky barrier potential. Computed resistivities in the presence of a barrier are only 3.5:1 to 4:1 above Landauer limits.**

***Index Terms* — Contact resistivity, Landauer limit, metal semiconductor junctions, Schottky barrier, transmission probability.**

I. Introduction

Low-resistivity metal-semiconductor contacts are fundamental to the scaling of transistors in both nm VLSI and sub-mm-wave/THz applications [1, 2]. In high-frequency transistors, the conductivity and operating current densities of contacts must both increase in proportion to the square of operating frequency. Similar scaling is required of MOSFET source/drain contacts in VLSI because of decreasing S/D contact pitch and of increasing drain current per unit gate width. Improved contacts are under development for both group IV and III-V compound semiconductors. Degenerate active carrier concentration, Schottky barrier height, and semiconductor surface preparation are the primary factors that determine contact resistivity [3, 4, 5]. Contact resistivity is determined by finite values of transmission probability *T*, electron velocity and density of available conduction states. For *T* = 1, this lower limit is known as the Landauer quantum conductivity limit. Here we compare published InGaAs and InAs contact resistivity data with calculations of contact resistivity both in the presence of an interfacial Schottky barrier and in the Landauer limit. We find that experimental contact resistivities for *n*-$In_{0.53}Ga_{0.47}As$ and *n*-InAs lie within 2.5:1 of calculated resistivities given generally accepted values of Schottky barrier potential. Further, computed resistivities in the presence of a barrier are only 3.5:1 to 4:1 above Landauer limits.

II. Current Density and Contact Resistivity Calculations

We first present the methods used here to calculate contact resistivity. Assuming conservation of transverse momentum and total energy, the net current density crossing the metal-semiconductor interface is [6]

$$J = \frac{2q}{(2\pi)^3} \int_{k_{sx}=-\infty}^{k_{sx}=\infty} \int_{k_{sy}=-\infty}^{k_{sy}=\infty} \int_{k_{sz}=0}^{k_{sz}=\infty} v_{sz} \cdot (f_s - f_m) \cdot T \cdot dk_{sx} dk_{sy} dk_{sz} \,, \tag{1}$$

where k_{sx} , k_{sy} and k_{sz} are the wave vectors in the semiconductor in x , y and z (transport) directions, v_{sz} is the z component of the electron group velocity in the semiconductor, and T is the interface transmission probability. The Fermi function in the semiconductor is $f_s = (1+\exp((E-E_{fs})/kT))^{-1}$, while that of the metal is $f_m = (1+\exp((E-E_{fm})/kT))^{-1}$, where E is the total electron energy, E_{fs} and E_{fm} are the Fermi energies in the semiconductor and in the metal, and $E_{fs} - E_{fm} = qV$, where V is the applied bias voltage.

The contact resistivity ρ_c is $(dV/dJ)\big|_{V=0}$ and hence is

$$\frac{1}{\rho_c} = \frac{2q^2}{(2\pi)^3 kT} \times \int_{k_{sx}=-\infty}^{k_{sx}=\infty} \int_{k_{sy}=-\infty}^{k_{sy}=\infty} \int_{k_{sz}=0}^{k_{sz}=\infty} \frac{v_{sz} \cdot T \cdot \exp\left(\frac{E-E_{fs}}{kT}\right)}{\left(1+\exp\left(\frac{E-E_{fs}}{kT}\right)\right)^2} dk_{sx} dk_{sy} dk_{sz} \,. \tag{2}$$

We approximate the metal's $E-k$ dispersion relationship as a single parabolic band with conduction band energy E_{cm} . For a semiconductor with parabolic energy dispersion, the total electron energy is

$$E = q\phi_R + \frac{\hbar^2}{2m_s}(k_{sx}^2 + k_{sy}^2 + k_{sz}^2) \,, \tag{3}$$

where $q\phi_R = E_{cs} - E_{cm}$ is the difference between the metal and semiconductor conduction band energies, m_s is the electron mass in the semiconductor. Energies are computed relative to E_{cm} .

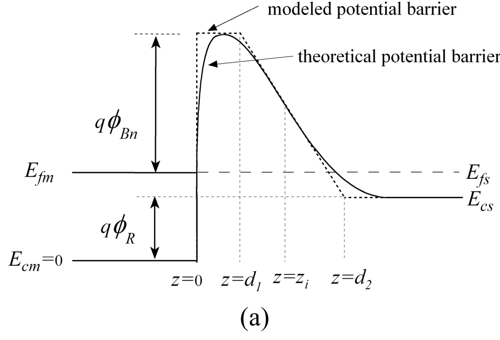
The electron group velocity is given by

$$v_{sz} = \frac{1}{\hbar}\frac{\partial E}{\partial k_{sz}} = \frac{\hbar k_{sz}}{m_s} \,. \tag{4}$$

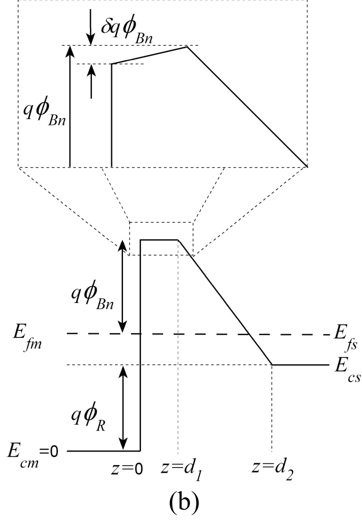
From equations (2), (3) and (4),

$$\frac{1}{\rho_c} = \frac{2q^2\hbar}{(2\pi)^3 m_s kT} \times \int_{k_{st}=-\infty}^{k_{st}=\infty} \int_{k_{sz}=0}^{k_{sz}=\infty} \int_{\theta=0}^{\theta=2\pi} \frac{T \cdot \exp\left(\frac{E-E_{fs}}{kT}\right)}{\left(1+\exp\left(\frac{E-E_{fs}}{kT}\right)\right)^2} k_{st} dk_{st} k_{sz} dk_{sz} d\theta \,, \tag{5}$$

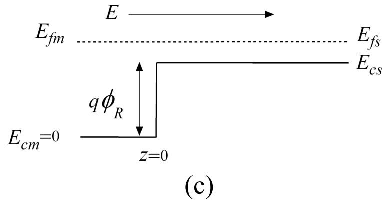
where $k_{st}^2 = k_{sx}^2 + k_{sy}^2$ and $dk_{sx} dk_{sy} = k_{st} dk_{st} d\theta$,



(a)



(b)



(c)

Figure 1: (a) Schematic of the theoretical and modeled potential barrier. (b) Detailed schematic of the modeled potential barrier. (c) Schematic of a step potential energy barrier.

$$\frac{1}{\rho_c} = \frac{q^2\hbar}{2\pi^2 m_s kT} \int_{k_{st}=-\infty}^{k_{st}=\infty} \int_{k_{sz}=0}^{k_{sz}=\infty} \frac{T \cdot \exp\left(\frac{E-E_{fs}}{kT}\right)}{\left(1+\exp\left(\frac{E-E_{fs}}{kT}\right)\right)^2} k_{st}dk_{st}k_{sz}dk_{sz} . \quad (6)$$

Equation (6) gives the contact resistivity for the case of parabolic bands.

For a semiconductor with non-parabolic energy dispersion, the total electron energy is approximately [7]

$$(E - q\phi_R)(1+\alpha(E-q\phi_R)) = \frac{\hbar^2}{2m_s}(k_{st}{}^2 + k_{sz}{}^2) , \quad (7)$$

from which we find

$$E = q\phi_R + \frac{1}{2\alpha}\left[\sqrt{1+\frac{2\alpha\hbar^2(k_{st}{}^2+k_{sz}{}^2)}{m_s}} - 1\right] , \quad (8)$$

where α is the non-parabolicity factor. The group velocity is then

$$v_{sz} = \frac{1}{\hbar}\frac{\partial E}{\partial k_{sz}} = \frac{\hbar k_{sz}}{m_s}\left(1+\frac{2\alpha\hbar^2(k_{st}{}^2+k_{sz}{}^2)}{m_s}\right)^{-1/2} , \quad (9)$$

from which we find the contact resistivity given non-parabolic bands,

$$\frac{1}{\rho_c} = \frac{q^2\hbar}{2\pi^2 m_s kT} \times \int_{k_{st}=-\infty}^{k_{st}=\infty} \int_{k_{sz}=0}^{k_{sz}=\infty} \frac{T \cdot \exp\left(\frac{E-E_{fs}}{kT}\right)}{\left(1+\exp\left(\frac{E-E_{fs}}{kT}\right)\right)^2} \frac{k_{st}dk_{st}k_{sz}dk_{sz}}{\left(1+\frac{2\alpha\hbar^2(k_{st}{}^2+k_{sz}{}^2)}{m_s}\right)^{1/2}} . \quad (10)$$

A. Calculation Of Transmission Probability,

The Wentzel-Kramers-Brillouin (WKB) approximation is frequently used to calculate metal-semiconductor interface transmission probability [8]. This approximation breaks down at the regions close to the maximum of the potential energy barrier and neglects quantum mechanical reflection at the metal-semiconductor interface. These limitations are important in modern heavily-doped junctions where the tunneling probability approaches unity.

Here we have calculated the exact transmission coefficient, including quantum mechanical reflection and valid in all energy ranges. From the combined effects of depletion region electrostatics and image-force, the semiconductor band energy E_{cs} is first computed as a function of position. This is then fit to a piecewise-linear approximation (fig. 1(a)). For $0 < z < d_1$, E_{cs} is fit to the peak barrier potential. In the region $d_1 < z < d_2$, the magnitude $\mathcal{E}_{\max}$ and location ($z = z_i$) of the point of maximum field in the depletion region is first calculated. E_{cs} is then approximated for $d_1 < z < d_2$ with a first-order linear potential fit of field $\mathcal{E}_{\max}$ passing through the point $z = z_i$.

Schrodinger's equation is then solved using Airy functions. An infinitesimal gradient $\delta q\phi_{Bn}$ is introduced in the $0 < z < d_1$ region (fig. 1(b)) as it facilitates the use of Airy functions in this region. The Airy function solutions are valid in all the energy ranges [9] i.e. $q\phi_R < E < \infty$ making the calculations less cumbersome. If a barrier with constant potential energy was chosen for this region ($0 < z < d_1$), it would require solutions of Schrodinger equations for $q\phi_R < E < q\phi_{Bn}$, $E = q\phi_{Bn}$ and $E > q\phi_{Bn}$, making the calculations tedious. The detailed calculations of transmission probability are presented in [10].

It must be noted that the present calculations neglect band gap narrowing arising from heavy doping. Treatment of the metal $E-k$ dispersion relationship as a single parabolic band introduces errors in the metal-semiconductor interface reflection probability. This limitation should be addressed in future work.

B. Landauer Contact Resistivity

In modern III-V transistors serving high-frequency applications, under the contacts a semiconductor doping of 5×10^{19} cm^{-3} to 1×10^{20} cm^{-3} is typical. For $In_{0.53}Ga_{0.47}As$ and InAs, where ϕ_{Bn} is small (<0.2 V), the associated depletion depths are 1 nm or less, and tunneling probability through the barrier potential--even if the barrier energy is positive-- is high. In such cases, contact resistivity remains nonzero because of quantum mechanical reflection at the interface, finite electron velocity and finite density of energy states available for electron transport.

Contact resistivity can be expressed as the inverse of the product of the density per unit area, conductivity $q^2/\pi\hbar$, and transmission probability T of available 1-D Landauer conduction channels. In the Landauer limit, T = 1 and $\sigma_c = (q^2/\hbar)(3/8\pi)^{2/3}\cdot\sum_{i=1}^{g}(m_{xi}m_{yi}/m_{zi}^2)^{1/6}n_{ei}^{2/3}$, where g is the # of valleys, m_{xi}, m_{yi}, m_{zi} the masses in the *x, y* and *z* (transport) directions, and n_{ei} the electron concentration in the ith valley. $\sigma_c = (q^2/\hbar)(3/8\pi)^{2/3}n^{2/3}$ for Γ-band (III-V) semiconductors, while for contacts to (100) Si, $\sigma_c = (q^2/\hbar)(3/8\pi)^{2/3}(n/6)^{2/3}(4(m_l/m_t)^{1/6}+2(m_t/m_l)^{1/3})$.

III. RESULTS AND DISCUSSION

Figure 2 compares calculated contact resistivities for parabolic and non-parabolic bands for *n*-InAs. A step-potential barrier (fig. 1(c)) was assumed. Resistivities lie slightly above Landauer limits because of interface quantum reflectivity; parabolic and non-parabolic bands show differing $(E_{fs}-E_{cs})$ and hence differing interface reflectivity. At a given electron concentration, Landauer contact resistivities are slightly lower in Si than in Γ-minima InAs because of the multiple band minima and the anisotropic bands.

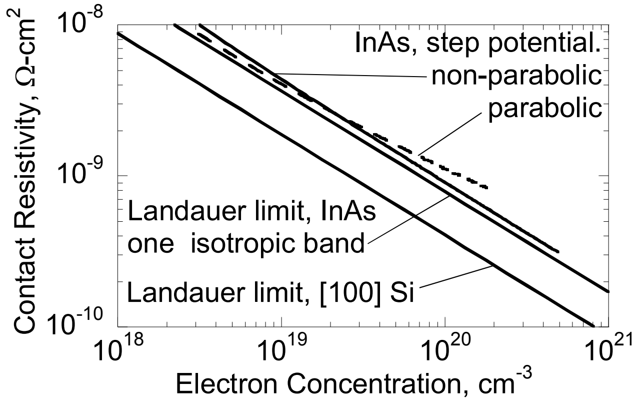


Figure 2: Landauer contact resistivity: for a single isotropic band and for (100) Si, and resistivity of InAs contact with a step-potential interface.

For Schottky tunnel barriers (fig. 1(b)), T was calculated assuming parabolic bands. Contact resistivities were calculated (fig. 3) and compared with published experimental data for *n*-$In_{0.53}Ga_{0.47}As$, *p*-$In_{0.53}Ga_{0.47}As$, *n*-InAs and *p*-InAs, as a function of electron/hole concentration and barrier height ϕ_B. We had earlier reported ultra-low contact resistivities obtained for *n*-InAs, *n*-$In_{0.53}Ga_{0.47}As$ and *p*-$In_{0.53}Ga_{0.47}As$ [11, 12, 13]. The contact resistivities were (0.6 ± 0.4) × 10^{-8} Ω-cm^2, (1.1 ± 0.5) × 10^{-8} Ω-cm^2 and (0.6 ± 0.5) × 10^{-8} Ω-cm^2 for *n*-InAs, *n*-$In_{0.53}Ga_{0.47}As$ and *p*-$In_{0.53}Ga_{0.47}As$, respectively, which are the lowest contact resistivities reported to date for these semiconductors.

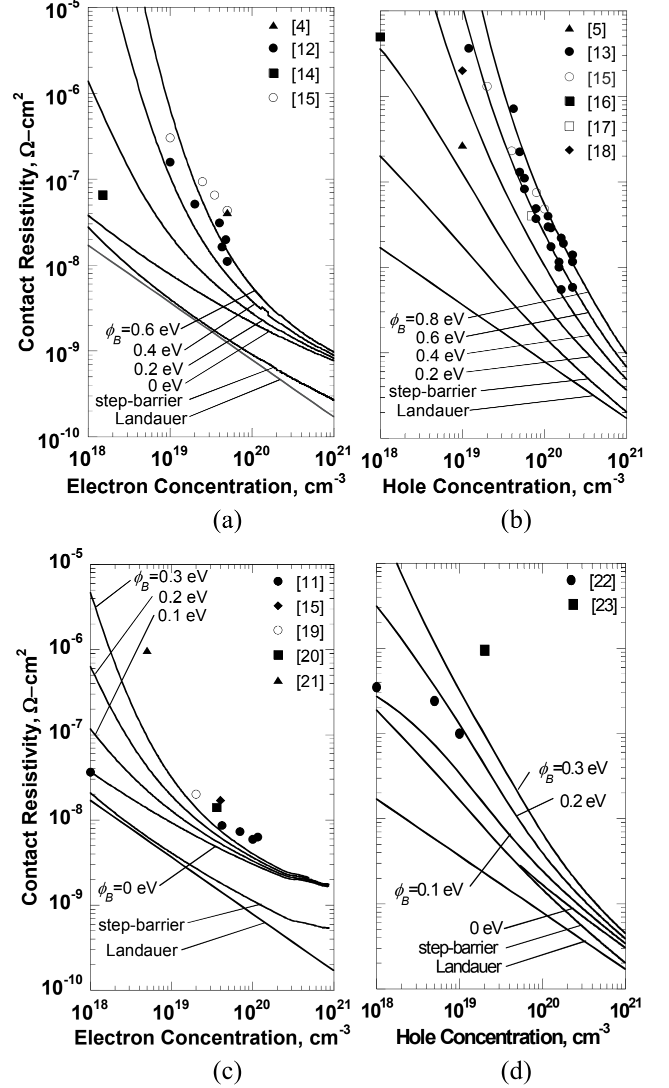


Figure 3: Calculated dependence (represented by lines) of contact resistivities (ρ_c) on bulk electron/hole concentration and Schottky barrier height (ϕ_B) for (a) *n*-$In_{0.53}Ga_{0.47}As$ (b) *p*-$In_{0.53}Ga_{0.47}As$ (c) *n*-InAs and (d) *p*-InAs. Experimental data from the literature is shown for comparison.

Computed contact resistivities show the expected strong dependence on electron/hole concentration and on ϕ_B. Even for contacts formed by *in-situ* deposition of refractory metals [11, 12, 13], where interfaces are expected to have an oxide/contaminant free metal-semiconductor interface, experimental resistivities of *n*-type contacts lie above theory given generally reported values of barrier potential. Measured contact resistivity to *n*-$In_{0.53}Ga_{0.47}As$ at 5×10^{19} cm^{-3} electron concentration is 2.3:1 higher than calculated assuming ϕ_B = 0.2 eV, while measured contact resistivity to *n*-InAs at 10^{20} cm^{-3} electron concentration is 1.9:1 higher than calculated assuming ϕ_B = 0 eV. In contrast, measured contact resistivity to *p*-

$In_{0.53}Ga_{0.47}As$ at 2.2×10^{20} cm^{-3} hole concentration correlates well with theory if $\phi_B = 0.6$ eV is assumed.

Calculations also show the degree to which the Schottky barrier increases contact resistivity. Computed contact resistivity for n-$In_{0.53}Ga_{0.47}As$ at 5×10^{19} cm^{-3} electron concentration and $\phi_B = 0.2$ eV is only 3.9:1 larger than the Landauer limit, while computed resistivity of n-InAs at 10^{20} cm^{-3} electron concentration and $\phi_B = 0$ eV is only 3.6:1 larger than Landauer limit. For p-$In_{0.53}Ga_{0.47}As$ at 2.2×10^{20} cm^{-3} hole concentration and $\phi_B = 0.6$ eV, computed resistivity lies 13:1 above the Landauer limit; the tunneling probability remains low.

Assuming that such electron/hole concentration levels can be made feasible, contact resistivity will approach 10^{-9} Ω -cm^2 as electron/hole concentration is increased to $\sim10^{21}$ cm^{-3}, both because of increased Landauer conductivity and increased contact transmission probability. Noting the curves for $\phi_B = 0$ eV in fig. 3(a) and 3(c), it is seen that for n-$In_{0.53}Ga_{0.47}As$ and n-InAs contacts, because of interface quantum reflectivity, contact resistivities do not drop far below 10^{-9} Ω-cm^2 even for electron concentration approaching 10^{21} cm^{-3}.

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