Scaling of nano-Schottky-diodes

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A generally applicable model is presented to describe the potential barrier shape in ultra small Schottky diodes. It is shown that for diodes smaller than a characteristic length $l_c$ (associated with the semiconductor doping level) the conventional description no longer holds. For such small diodes the Schottky barrier thickness decreases with decreasing diode size. As a consequence, the resistance of the diode is strongly reduced, due to enhanced tunneling. Without the necessity of assuming a reduced (non-bulk) Schottky barrier height, this effect provides an explanation for several experimental observations of enhanced conduction in small Schottky diodes.

We only model the barrier shape in the semiconductor; the SBH $\varphi_B$ is accounted for in boundary conditions and is considered as a given quantity. For simplicity, the depletion approximation is adopted, which is valid for a wide range of realistic parameters. Moreover, the space charge region is assumed to be homogeneously charged, an assumption that will be discussed later. Solving the Poisson equation in n-type silicon with the boundary condition that the charge on the sphere cancels the total charge in the space charge region, we find for $0 \leq x \leq w$,

$$\frac{e}{kT} \cdot V(x) = \frac{1}{2 L_D^2} \left( (a+w)^2 - 2(a+w)^3 - \frac{(a+x)^2}{3} \right),$$

where $x$ is the radial distance from the interface, $w$ the depletion width and $L_D = \sqrt{\varepsilon_s kT/(e^2 N_d)}$ the Debye length. The zero-point of the potential is chosen in the semiconductor bulk. The value of $w$ is fixed by the second boundary condition $V(0) = V_s$, where $V_s$ is the total potential drop over the space charge region and satisfies $V_s = (\varphi_B - \varphi_s)/e - V$ (with $\varphi_s = E_c - E_f$). Eq. (1) is valid for small bias voltage $V$. The limited validity of the depletion approximation at finite temperatures only affects the tail of the barrier (where $|V(x)| \lesssim kT$), which is unimportant for the transport properties. From the equation, it can be seen that the characteristic length scale of this system is

$$l_c \stackrel{\text{def}}{=} L_D \sqrt{2eV_s/kT} = \sqrt{\frac{2eV_s}{eN_d}}.$$

By comparing the diode size $a$ to $l_c$ we can decide whether the diode is ‘small’ or ‘large’. In the lower right inset of Figure 1 the value of $l_c$ is plotted versus doping concentration $N_d$.

An important quantity for electrical transport is the Schottky barrier thickness. In Figure 1, the barrier full width at half maximum (FWHM, $x_{1/2}$) calculated from Eq. (1) is plotted as a function of diode size $a$. From the figure it is clear that for $a \gg l_c$ the value of $x_{1/2}$ approaches a constant, which was expected for a large diode. Indeed, for $a \gg l_c$, Eq. (1) reduces to
FIG. 1: Plot of the calculated barrier FWHM $x_{1/2}$ as a function of diode size $a$ (based on Eq. 1), both in units of $l_c$. The dashed lines represent the asymptotic values for $a \gg l_c$ (conventional diode) and $a \ll l_c$ (new regime) respectively. The lower right inset is a plot of $l_c$ as a function of doping level $N_d$ in silicon ($\varepsilon_s = 11.7$) for $\varphi_B = 0.67$ eV and $T = 300$ K. The upper left inset schematically shows the model system, a metallic sphere embedded in semiconductor.

FIG. 2: The solid lines are contours of the barrier FWHM for various disc-shaped contacts (see inset; radii ranging from 30 nm (a) to infinite (c)), taken from a numerical solution of the Poisson equation in silicon. It clearly shows the contact size dependence for contact radii smaller than $l_c \approx 750$ nm. The dashed lines are the FWHM-contours of the barrier for the three smallest diodes, neglecting the screening effect of the semiconductor space charge region. The inset indicates the plane of cross-section shown in the figure.

$V(x) = -\frac{2N_s}{\varepsilon_s}(x-w)^2$, which is the well-known textbook result for band bending in the depletion approximation for an infinitely large diode. Both the depletion width $w = \sqrt{(2\varepsilon_s/eN_s)V_s}$ and $x_{1/2}$ are in that regime independent of $a$.

Figure 1 shows that for $a \lesssim l_c$ the value of $x_{1/2}$ is no longer constant, but decreases with decreasing $a$. For $a \ll l_c$ it approaches $x_{1/2} = a$, i.e. the barrier thickness equals the diode size. This also follows from Eq. 1, which reduces to $V(x) = V_s \cdot a/(a + x)$ for $a \ll l_c$ and $x \ll w$ (that is, close to the interface). Note that this is exactly the potential due to the charged sphere only. In this regime, the effect of the semiconductor space charge on the barrier shape and thickness can be neglected. This can be understood from the fact that the screening due to the space charge region takes place on a length scale $l_s$, as in conventional (large) diodes. However, from Gauss’s law it follows that any charged object of typical size $d < \infty$ in a dielectric medium gives rise to a potential that behaves roughly as $V(r) \propto d/r$. This Coulomb potential can be further screened by the formation of a space charge layer of opposite sign, but that additional screening can be neglected if $d \ll l_c$. This observation holds for any interface with typical dimensions much smaller than $l_c$.

In a geometry that can actually be fabricated, the Poisson equation must be solved numerically. We have done this for n-doped silicon ($N_d = 10^{15}$ cm$^{-3}$) in contact with metallic circular disks of various radii. In all further calculations $\varphi_B = 0.67$ eV was used, which is the barrier height of the CoSi$_2$/Si(111)-interface. Figure 2 shows the FWHM-contours of the barriers as resulting from these calculations. Also shown are the FWHM-contours of the barrier due to the metallic contacts only, illustrating the negligible effect of the space charge region on the barrier thickness in very small diodes.

To study the effect of the reduced barrier width on the transport properties of a small Schottky diode, a transmission coefficient $T(E, V)$ was obtained for the barrier shape from Eq. 1. This was done in a one-dimensional fully quantum mechanical calculation. Note that $T(E, V)$ is implicitly dependent on temperature and doping level, because these quantities influence the position of the Fermi-level in the bulk semiconductor. The current density is then given by

$$J(V) \propto \int_0^\infty T(E, V)[f(\varphi_s + E) - f(\varphi_s + E + V)] dE,$$

from which it follows that the zero bias differential conductance satisfies

$$\frac{dJ}{dV}|_{V=0} \propto -\int_0^\infty T(E, V)f'(\varphi_s + E) dE.$$

Here, $f$ is the Fermi-Dirac distribution function and $E$ the energy above the semiconductor conduction band edge. Transport due to electrons at energies below the barrier maximum ($E < V_s$) is regarded as tunneling, while for $E > V_s$ we speak of thermionic emission. Obviously, the contribution of thermionic emission is almost independent of the barrier thickness, while tunneling is strongly dependent on the barrier thickness.

In Figure 3, the calculated zero bias differential conductance is plotted as a function of diode size $a$ for several values of $N_d$. For $a \gtrsim l_c$ this quantity is independent
I. Identifying behavior of the diode.

When the diode size decreases, the reverse current eventually becomes significant. This is because the potential barrier reduces in height and width, which leads to an increase in the reverse current. In extremely small diodes, this reverse current may even exceed the forward current, effectively reversing the direction of current flow.

II. Calculated IV curves for various diode sizes.

The IV curves for different diode sizes are shown in Figure 4. The characteristics of these curves change drastically with decreasing diode size. The curves of the larger diodes have a shape that is qualitatively similar to the IV curve for the infinite diode. However, as the diode size decreases, the curves become more exponential, with the tunnel current becoming dominant at lower voltages.

III. Qualitative changes in IV curves.

As the diode size decreases, the IV curve shape changes from a more linear to an exponential form. This is due to the increased influence of tunneling, which becomes the dominant contribution to the conduction of the diode, when the dopant resides close to the interface.

IV. Calculation of IV curves.

Our calculations (Fig. 4) show that the IV curve shape changes from a linear to an exponential form as the diode size decreases. For smaller values, the tunnel current starts to increase rapidly, eventually leading to a strong increase of the total conduction.

V. Discussion.

In conclusion, we have shown by means of a simple electrostatic argument that the Schottky barrier thickness becomes a function of the diode size for small diodes (e.g., smaller than $l_c \approx 80$ nm for $N_d = 10^{17}$ cm$^{-3}$). Consequently, the contribution of tunneling to the total conduction is greatly enhanced in small diodes. This effect explains several experimental results, without the assumption of a reduced SBH. Moreover, small diodes show IV-curve shapes that qualitatively differ from those of conventional diodes.

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