Influence of the band bending parameter on the current – voltage characteristics

Influence of the band bending parameter $b$ on the current density-voltage characteristics, calculated according to Eq. (13), using $\varphi_b = 1$ V. The transition from the exponential to the linear regime shifts in voltage. The current in the transition and linear regimes spans over almost 9 orders of magnitude for a variation $b$ from 0 to 0.5 V. This indicates that a correct value for $b$ is essential for application of Eq. (12) to real devices.

Derivation of the band bending parameter

Using Eq. (5) and its approximation Eq. (6) in the article of Simmons [J. Phys. Chem. Solids 32, 1987 (1971)], the conduction band $E_c(x)$ for an Ohmic electron contact at $x = 0$ can be approximated as

$$E_c(x) = kT \ln\left(\frac{q^2 N_e x^2}{2 kT e}\right).$$

The derivative is
\[
\frac{dE_c}{dx} = \frac{2kT}{x}.
\]  
(S2)

The band bending parameter \( b \) can be found by taking the tangent at \( x = L \), described by

\[
f(x) = (x - L)\frac{dE_c}{dx}\bigg|_{x=L} + E_c(L),
\]  
(S3)

and taking the intercept of \( f(x) \) with the energy axis at \( x = 0 \). This yields \( f(0) = qb \), giving

\[
qb = E_c(L) - L\frac{dE_c}{dx}\bigg|_{x=L} = kT \ln\left( \frac{q^2 N_c L^2}{2kT\varepsilon} \right) - 2kT,
\]  
(S4)

resulting in the expression for the band bending parameter \( b \) according to

\[
b = \frac{kT}{q} \left[ \ln\left( \frac{q^2 N_c L^2}{2kT\varepsilon} \right) - 2 \right].
\]  
(S5)

**Figure:** Conduction band for \( N_c = 3\times10^{26} \text{ m}^{-3} \), \( L = 100 \text{ nm} \), \( T = 295 \text{ K} \), and \( \varepsilon = 3\varepsilon_0 \). This gives \( b = 0.27 \text{ V} \). The approximation [Eq. (S1)] is very good for an Ohmic contact and is almost indistinguishable from the exact solution, which also exactly corresponds to the numerical result.
Current density-voltage characteristics for a range of temperatures plotted on a semi-logarithmic scale (a), and a double-logarithmic scale (b). Device parameters are: $\varphi_b = 0.5$ V, $N_v = 3 \times 10^{26}$ m$^{-3}$, $L = 100$ nm, and $\varepsilon = 3\varepsilon_0$. Mobility was varied with temperature using an Arrhenius temperature dependence with an activation energy of 0.4 eV. The dashed lines are the analytically calculated characteristics for the sum of drift and diffusion. The band bending parameter $b$ was calculated according to Eq. (13). The solid lines represent numerical simulations with the exactly the same parameters (note that band bending is taken into account implicitly in the numerical simulation).
Variation of the layer thickness, J-V characteristics plotted on a double-logarithmic scale. The analytical description is in agreement with the simulations for all layer thicknesses. The band bending parameter in the analytical calculations causes the transition from a $1/L$ thickness dependence to a $1/L^3$ layer-thickness dependence for the diffusion current. Therefore, with the correct band bending parameter [Eq. (13)], the diffusion current can connect to the space-charge-limited drift current [Eq. (1)], which also has a $1/L^3$ thickness dependence.

The device parameters are: $\phi_b = 0.5$ V, $\mu = 1 \times 10^{-9}$ m$^2$/Vs, $N_v = 3 \times 10^{26}$ m$^{-3}$, $T = 295$ K, and $\varepsilon = 3\varepsilon_0$. The dashed lines are the analytically calculated characteristics for the sum of drift and diffusion. The band bending parameter $b$ was calculated according to Eq. (13). The solid lines represent a numerical simulations with the exactly the same parameters.
Influence of a small barrier at the injecting contact

Numerically-simulated current density-voltage characteristics for a small barrier $\phi_a$ at the anode side, which is the hole injecting contact. The barrier at the cathode side, $\phi_b$, was kept fixed at 1 V. The other parameters are $\mu = 1 \times 10^{-9}$ m$^2$/Vs, $N_v = 3 \times 10^{26}$ m$^{-3}$, $L = 100$ nm, $T = 295$ K, and $\varepsilon = 3\varepsilon_0$. The characteristics are hardly influenced up to $\phi_a = 0.2$ V, for larger barriers the contact cannot supply enough carriers to maintain the space-charge-limited current and thus the current decreases.
Layer-thickness dependence of the current – voltage characteristics

Numerically-simulated current density-voltage characteristics for different layer thicknesses (a). Multiplication of the current density $J$ with the layer thickness $L$ results in collapsing of the low-voltage, diffusion-dominated regime onto a single curve (b). This shows that the layer-thickness dependence of the diffusion current [Eq. (12)] is correct: the current scales with $1/L$. At higher voltages (around the built-in voltage), the thickness dependence of the diffusion current increases. In the analytical expression, this is due the thickness dependence of the band bending parameter $b$. For voltages well above the built-in voltage, the space-charge-limited drift current becomes dominant and the current scales with $1/L^3$, as expected from Eq. (1).
Detection limit of the measurement setup

To indicate the detection limit of our setup, we recorded I-V scans without placing a sample in the setup. We have plotted also the PFO diode from Fig. 4, to show that the measurement extends down to the detection limit of about 100 pA.