MODELING LOCALIZED STATES AND BAND BENDING EFFECTS ON ELECTRON EMISSION ION FROM GaAs*

D. A. Dimitrov, C. Nieter, Y. Choi, Tech-X Corp., Boulder, CO 80303, USA
I. Ben-Zvi, J. Smedley, T. Rao, BNL, Upton, NY 11973, USA
I. Bazarov, S. Karkare, W. Schaff, CLASSE, Cornell University, Ithaca, NY 14853, USA

Abstract

High acceptor doping of GaAs and (Cs, O) surface coating leads to downward band bending terminating with effective negative electron affinity surface. The periodicity breaking at the surface together with the formed potential leads to one or more localized states in the band bending region together with effective Fermi level pinning. We report results on how to calculate the band bending potential, the Fermi level pinning, and localized states as functions of GaAs p-doping density, surface density of states, and temperature. We also consider how these surface properties affect electron emission.

INTRODUCTION

High-average current and high-brightness electron beams are needed in advanced applications such as ultra-high Free-Electron Lasers, electron cooling of hadron accelerators, and Energy-Recovery Linac light sources. Semiconductor cathodes, such as negative electron affinity GaAs-based cathodes, are known [1] to have good quantum efficiency (QE) (10% achieved experimentally), low thermal emittance with prompt response time [2], and are candidates to achieve high average current up to 100 mA.

However, how to design, fabricate, and reliably operate semiconductor cathodes at high average current (reaching 100 mA) still represents a major problem. Some of the most important effects to understand are related to surface space charge region, controlling the electron affinity and band bending as a function of surface properties and charge propagation to the surface [3, 4].

In addition to experiments, simulations provide a complementary way to efficiently explore relevant parameter sets. Moreover, they allow us to obtain data on properties that are currently not accessible through experiments or very difficult to measure. For example, the energy distribution of electrons inside the cathode material in the region of the emission surface is directly accessible in the simulations but very difficult to measure in experiments. Producing high fidelity simulations data of semiconductor cathode properties depends on accurate modeling of the surface space-charge region. Specifically, the calculation of the band bending region (BBR) energy profile, determination of Fermi level pinning (e.g. for GaAs cathodes), development of localized electron levels with emission from them, and how the electron affinity depends on these properties significantly affect electron emission.

Emission from localized states has been shown to contribute to the observed energy distribution of electrons from GaAs and one approach was proposed to explain it [3] that depends on specific properties of the potential across the GaAs-vacuum interface. Similar effects were considered for emission from diamond but the model developed was based on a different surface potential [5].

We have already done simulations with a surface band bending profile that uses a quadratic approximation [6]. Here, we provide a general approach for calculation of the band bending profile and the Fermi level pinning for GaAs.

BAND BENDING AND LOCALIZED STATES

The surface band bending arises as a consequence of the space charge region that develops as a result of the symmetry breaking and appearance of surface states. The electrostatic potential in the band bending region (BBR) is determined from the solution of the Poisson equation:

$$\nabla \cdot (\varepsilon \nabla \phi) = q \left(n\left[\phi\right] - p\left[\phi\right] + N_A^-\left[\phi\right] - N_D^+\left[\phi\right] \right), \quad (1)$$

where $\varepsilon(\mathbf{r})$ is the dielectric constant, q is the fundamental charge, n and p are the electron and hole densities in the conduction and valence band, respectively, N_A^- and N_D^+ are the densities of ionized acceptor and donor impurities when present. Generally, all charge densities are non-linear functions of the potential. When periodicity is preserved in the emission surface, the resulting non-linear Poisson equation is effectively one-dimensional. For p-doped GaAs, when the donor density can be neglected and the acceptors are fully ionized, it has the form:

$$\frac{d^2U(x)}{dx^2} = \frac{q^2}{\varepsilon k_B T}\left(N_A - \frac{2N_V}{\sqrt{\pi}} F_{1/2}\left(\eta_V - U(x)\right)\right), \quad (2)$$

where $\eta_V = (E_V - E_F)/k_BT$ (with E_V the valence band maximum in bulk and E_F the Fermi level, k_B the Boltzmann constant and T the lattice temperature), $U(x) = q\phi(x)/k_BT$, $N_V = 2\left(\frac{m_{dh}k_BT}{2\pi\hbar^2}\right)^{3/2}$ with m_{dh} a hole-related effective mass, and $F_{1/2}(x) = \int_0^\infty \frac{\sqrt{u}}{1+e^{u-x}}du$. The boundary conditions imposed on the 1D non-linear Poisson equation are determined from the requirement of zero

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applied field in bulk:

$$\frac{dU}{dx}\left(x \to \infty\right) = 0,$$

and a given value at the semiconductor surface

$$U\left(x = 0\right) \equiv U_S \equiv q\phi_S / k_B T.$$

This 1D non-linear Poisson equation can be solved by a finite difference discretization and then using a Newton-Ralphson algorithm to find the roots of the resulting matrix equation.

In the case of non-degenerate semiconductors, $E_V + 3k_BT \leq E_F \leq E_C - 3k_BT$ where E_C is the minimum of the conduction band in bulk, the solution for the band bending potential can be expressed in the integral form:

$$\mathrm{sgn}\left(U_S\right) \int_{U(x)}^{U_S} \frac{du}{F\left(u,\, U_F\right)} = \frac{x}{L_D}, \qquad (3)$$

where

$$F\left(x, y\right) = \sqrt{e^y\left(e^{-x} + x - 1\right) + e^{-y}\left(e^x - x - 1\right)},$$

$U_F = \left(E_i - E_F\right)/k_BT$ with E_i the Fermi level for the intrinsic semiconductor (no ionized impurities), and $L_D = \sqrt{\frac{\varepsilon k_B T}{2q^2 n_i}}$ with n_i the conduction band electron density in the intrinsic case.

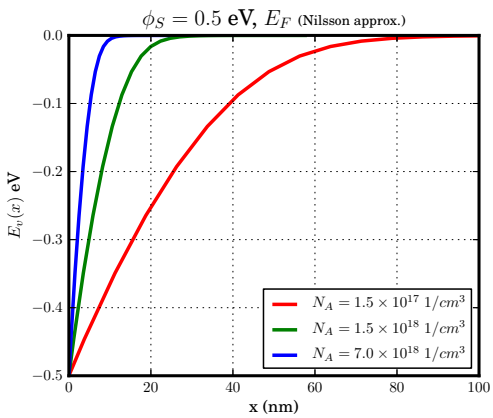

Figure 1: Calculated band bending energies as a function of acceptor doping for three different values. The band bending for $N_A = 7 \times 10^{18}$ cm^{-3} and $\phi_S = 0.5$ eV is in agreement with previously published data [3].

The value of the potential ϕ_S at the surface is determined from the requirement to satisfy charge neutrality. Since U_F is calculated from bulk properties as a function of temperature and bulk doping density, we can determine the band bending potential $U(x)$ by numerically solving Eq. (3). We have implemented a bisection algorithm to evaluate the integral in Eq. (3) and find its root for a given value of x. The value of $U(x)$ for the lower limit of the integral from the calculated root value represents the band bending potential at distance x from the GaAs surface. Results from the code are shown in Fig. 1 for three different acceptor doping densities and a pinned surface potential energy $q\phi_S = 0.5$ eV. The results demonstrate the importance to consider the nonlinear corrections since the band-bending profiles deviate from the initially assumed quadratic form. Moreover, we can now directly obtain the depth of the band bending potential in GaAs when varying the bulk acceptor density. Finally, the obtained band bending profile for $N_A = 7 \times 10^{18}\ cm^{-3}$ is in good agreement with previously published data [3].

For the results presented in Fig. 1, the Fermi level position was calculated from bulk properties using Nilsson's approximation (see [6] and references therein).

The value of the potential ϕ_S at the surface is determined from the requirement to satisfy charge neutrality. Moreover, at specific surface conditions for GaAs, the surface potential ϕ_S and the Fermi level are pinned. For

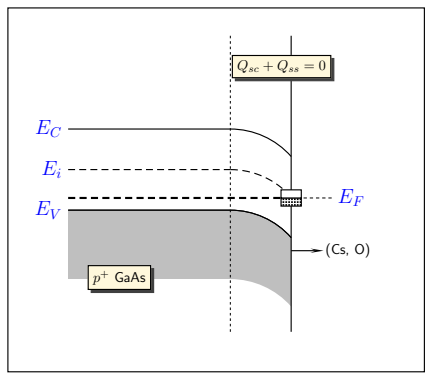

Figure 2: The Fermi pinning regime is reached when the band bending leads to overlap of the energy of the surface states (shown in the diagram with the partially filled rectangle) with the chemical potential E_F.

p-doped GaAs and downward band bending $\phi_S > 0$ at the surface and $\phi\left(x \to \infty\right) \to +0$ in bulk, the space-charge region is negatively charged since near the surface: $p\left(x\right) - N_A = p\left(x\right) - p_{bulk} < 0$. For this case, charge neutrality at the surface can be satisfied if there are surface donor states that are positively charged. The surface band bending ϕ_S is determined from the charge neutrality condition $Q_{ss}\left(\phi_S\right) + Q_{sc}\left(\phi_S\right) = 0$ where $Q_{ss}\left(\phi_S\right)$ is the total change density on surface states and $Q_{sc}\left(\phi_S\right)$ is the space-charge surface density $\left|Q_{sc}\left(\phi_S\right)\right| = \left|\varepsilon \frac{d\phi(x=0)}{dx}\right|$. For a given type of a surface donor state with density N_{sd}, Q_{ss} is determined from:

$$Q_{ss}\left(\phi_S\right) = qN_{sd}\left(1 - 1/\left(\exp\left(\beta\left(E_{sd} - E_F\right)\right) + 1\right)\right),$$

where E_{sd} is the energy of electrons on the surface state, determined by atomic properties and is at a given position (0.55 eV for GaAs) relative to the valence band maximum at the surface effectively making $E_{sd} - E_F$ a function of ϕ_S. The band bending potential determined from the charge neutrality condition is reached when $E_F \approx E_{sd}$

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as shown in Fig. 2. The plots in Fig. 3 indicate the onset of the Fermi level pinning for different N_A values and approaches to calculate E_F (the bottom right plot uses an exact numerical calculation for the Fermi level rather than the Nilsson approximation). From the plots at low bulk doping in Fig. 3, the Fermi level and ϕ_S are pinned for for $N_{sd} \geq 10^{12}$ cm^{-2} while for high doping, the pinning regime is reached for $N_{sd} \geq 10^{13}$ cm^{-2}. The Fermi level

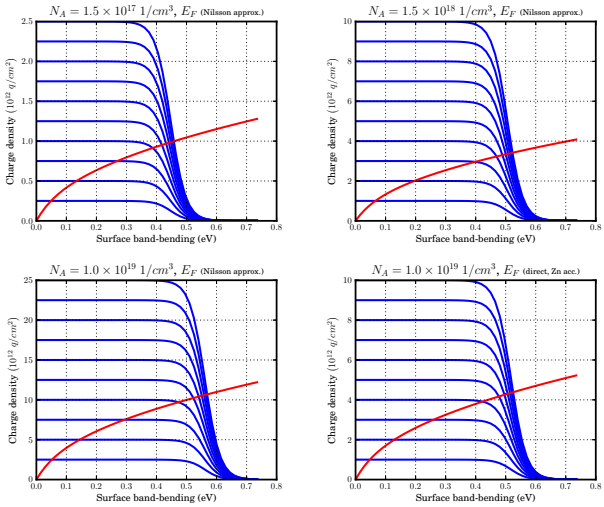

Figure 3: The intersection of each Q_{ss} curve (for a given surface state density N_{sd}) with the Q_{sc} curve for given doping concentration N_A determines the value of the surface band bending ϕ_S.

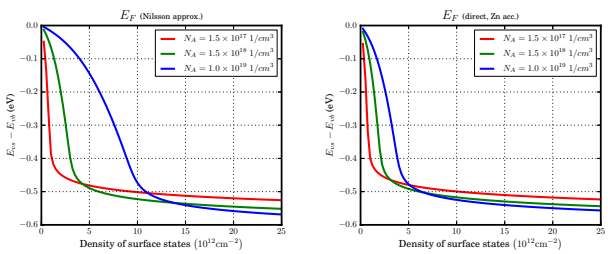

Figure 4: When the band bending leads to $E_F \approx E_{sd}$, the Fermi level at the surface changes only by $2.3k_BT$ per decade of surface state density. This is the regime of effective Fermi level pinning due to the small change of E_F with further increase of the surface density of states.

pinning regime is clearly revealed when we calculate ϕ_S as a function of the surface density of states for different bulk acceptor concentrations. Results from these calculations are shown in Fig. 4. In the pinning regime, the surface band bending ϕ_S changes little when further increasing the surface density of states N_{sd}. Note that the values for which the Fermi pinning regime starts, $N_{sd} \sim 10^{12}$ to 10^{13} cm^{-2} is still orders of magnitude smaller that the value 10^{15} cm^{-2} for the density of a complete monolayer of adatoms.

Finally, we briefly mention the importance of including emission from localized states that develop in the BBR. This effect was demonstrated in electron emission energy distribution data for GaAs [3]. The localized energy levels can be calculated by self-consistently solving the Schrödinger-Poisson equations in the BBR. We have prototyped an implementation to solve the Schrödinger-Poisson equations self-consistently and are currently investigating results from it with different emission surface potentials. Note, however, that depending on the boundary conditions imposed when solving the Schrödinger-Poisson equations, emission from quasi-stationary levels and electron lifetime on them has to be included in the calculations [3].

SUMMARY

We reported here results for calculation of the band bending region and pinning of the Fermi level in p-doped GaAs as a function of the acceptor doping concentration and the density of surface states. The results allow for accurate evaluation of the band bending in the surface space-charge region. The calculated band bending profiles can be used as input in codes to simulate charge transport and electron emission from semiconductor cathodes. Emission from localized states represents another important effect that is still to be properly integrated in photocathode simulations.

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