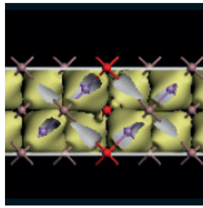



## Nonequilibrium Green's function method: Performance prediction of band-to-band tunneling devices in electron-only representation

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Band-to-band tunneling field-effect transistors (TFETs) have gained great interest since their switching behavior is not affected by the 60mV/decade limit of traditional FETs. This fact makes them promising candidates for low power electronics. The quantitative prediction of TFET performances requires self-consistent solutions of charge distributions and transport equations. The nonequilibrium Green's Function (NEGF) method is widely accepted as a method of choice for this purpose [1]. It is common, however, to consider charge contributions of the conduction and valence band as electron and holes separately [2]. Although it is known to fail for band-to-band tunneling devices [3], this concept is still applied in many TFET studies [4]. In this work, a numerically efficient charge self-consistent model is developed where only electrons are considered throughout all bands – including the deepest lying valence band. Comparison of the common electron-hole picture with the new method shows agreement in standard FETs and systematic deviations in TFETs. Predictions of critical transistor benchmarks such as the transconductance are unreliable in the electron-hole picture.

In band-to-band tunneling valence band electrons tunnel across the semiconductor band gap to the conduction band. A direct implementation of charge self-consistent models of this process with the re- sponse of all other electrons requires a numerically expensive discretization of all valence band ener- gies. In the NEGF method, however, the density of particles that are distributed in equilibrium can be solved by applying the residual theorem. With the Gaussian quadrature method, the numerical integration on the complex energy contour converges with only few tens of points [5]. The positive background ionic charge is calculated at equilibrium for every respective device structure. Electrons in nonequilibrium, i.e. those that face unequal lead distribution functions are still solved on the real energy axis. The free charge density of bulk silicon is illustrated in Fig. 1 when solved with the electron- only and the traditional electron-hole representa- tion. It can be seen that the electron-only method matches well with the standard one in cases without pronounced band-to-band tunneling.

The impact of the electron-only charge self- consistent model is easy to see in the example of a silicon ultra-thin body double-gate transistor. The ballistic transfer characteristics $I_d - V_{gs}\ at\ V_{ds} = 0.1V$ are presented in Fig. 2. The differences in the predicted performance of the traditional and new method can be understood in Fig. 3. The electron density in the bandgap (at positions around 10 nm) is considered as electrons only in the new method, whereas the traditional electron-hole method gives ambiguous charge prefactor assignements to it (in- dicated by the electron/hole delimiter line in Fig. 3). In consequence, the electrostatic potential around that position differs in the two methods which causes the transmission results (and with them the transfer characteristics) to differ as well (see Fig. 4).

We have developed a charge self-consistent model for quantum transport calculations in TFETs where standard charge self-consistent approaches that distinguish between electrons and holes fail. Although the new model enhances the predictive power of NEGF for band-to-band tunneling devices significantly, it keeps the numerical load virtually unaltered.

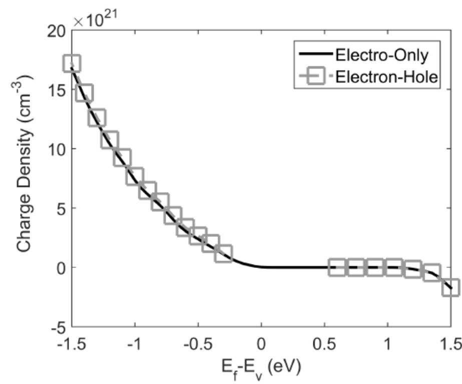


Fig. 1. The free charge density in bulk silicon is calculated in $sp3d5s^*$ tight-binding basis in the new method (black) and the traditional approach (gray). The x-axis indicates the distance between the Fermi level and the top valence band.

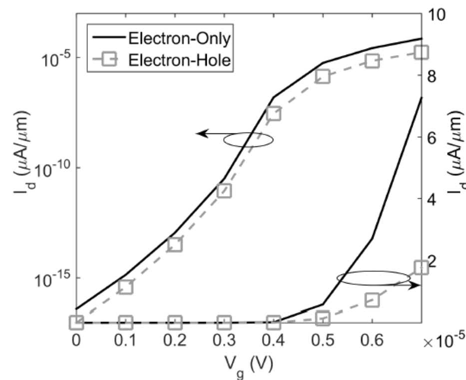


Fig. 2. Transfer characteristics $I_d - V_{gs}$ at $V_{ds} = 0.1V$ of a Si Ultra-thin body transistor with a double-gate contact of $L_g$=11 nm and a thickness of 1.6 nm.

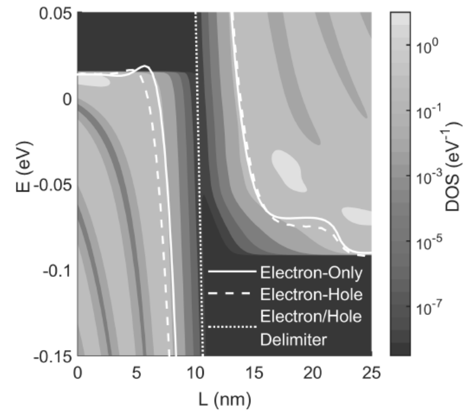


Fig. 3. Contour plot of the energy and position resolved density of states of the TFET simulated in Fig. 2 at $\Gamma$ point with the new electron-only method. The band-edge of the electron-hole picture and the delimiter line of electron and hole states are represented in dashed and dotted lines. The solid line shows the band profile of the electron-only picture.

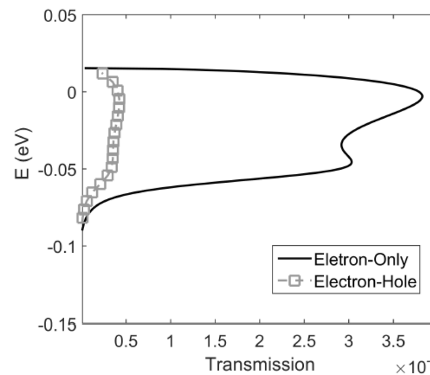


Fig. 4. Transmission at $\Gamma$ point of the device simulated in Fig. 2.

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