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Strong Quantization of Current-carrying Electron States in δ-layer Systems

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Abstract

We present an open-system quantum-mechanical real-space study of the conduction band structure and conductive properties of phosphorus δ-layers systems, interesting for their beyond-Moore and quantum computing applications. Recently it has been demonstrated [1] that an open-system quantum mechanical treatment gives much better match to ARPES measurements in highly-conductive highly-confined systems than the traditional (periodic or Dirichlet boundary conditions) approaches and allows accurate predictions of conductive properties of such systems from the first principles, i.e. by computing the quantum-mechanical flux. In order to evaluate size quantization effects on the conductivity of these systems, we consider two principal cases: nanoscale finite-width structures, used in transistors, and infinitely-wide structures, electrical properties of which are typically known experimentally. For devices widths $W < 10$ nm, quantization effects are strong and it is shown for the first time that the number of propagating modes determines not only the conductivity, but the distinctive spatial distribution of the current-carrying electron states. For $W > 10$ nm, the quantization effects practically vanish and the conductivity tends to the infinitely-wide device values.

Keywords: Si:P δ-layer systems, quantum transport, Contact Block Reduction method

1. Introduction

Highly conductive δ-layer systems, i.e. thin, high-density layers of dopants in semiconductors are actively used as a platform for exploration of the future quantum and classical computing when patterned in plane with atomic precision. Such structures, with the dopant densities above to the solid solubility limit have been shown to possess very high current densities and thus have a strong potential for beyond-Moore and quantum computing applications. However, at the scale important for these applications, i.e. devices with sub-20 nm physical gate/channel lengths and/or sub-20 nm widths, that could compete with the future CMOS [2], the conductive properties of such systems are expected to exhibit a strong influence of size quantization effects.

Recently it has been demonstrated in [1] that to accurately extract the conductive properties of highly-conductive, highly-confined systems, an open-system quantum-mechanical analysis is necessary. Such open-system treatment, that can be conducted for instance using the Non-Equilibrium Green's Function (NEGF) formalism.

In this work we employ an efficient computational implementation of NEGF that is called Contact Block Reduction and is summarized in [1]. A flow-chart of the algorithm implemented in our CBR simulator is shown in Fig. 1. For the self-consistent solution of the non-linear Poisson equation, we employed a combination of 1) automatic Fermi level determination using Neumann boundary conditions for the non-linear Poisson equation (where the uncertainty by energy is eliminated through the charge self-consistent coupling to the Schrodigner equation with Dirichlet and open-system boundary conditions [3]), 2) the open-system predictor-corrector approach[4] and 3) the Anderson mixing scheme[5]. In our previous work [1], we also developed and implemented in the CBR method a heuristic elastic electron-defect scattering for meso- and macroscopic scale. We note that other types of scattering effects are already taken into account

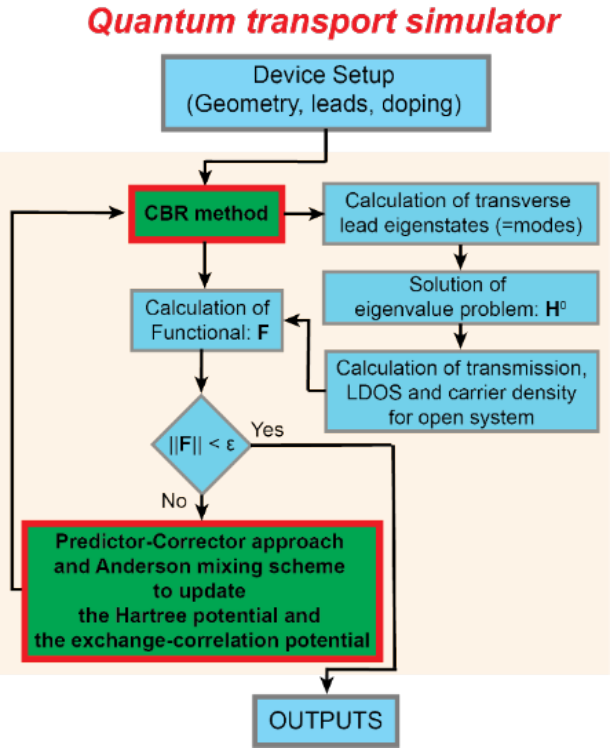

Figure 1: Flow chart of the self-consistent Contact Block Reduction method [9, 10, 4, 11, 5].

in our technique: the elastic electron-electron scattering is included through the self-consistent Hartree + LDA exchange-correlation terms that also reflect scattering on all electric fields inside the device. Scattering on discrete charged impurities in δ-layer systems has been analysed using the CBR method in [6]. Finally, as discussed in [1], inelastic scattering can be neglected at low temperature (4 K) since in Si:P-δ systems the phase-relaxation length l_ψ is larger than the mean free path l_m at low temperatures [7, 8]. Thus, all most relevant scattering effects at 4 K are taken into account by our computational scheme.

We demonstrate that for devices widths $W < 10$ nm, quantization effects are strong and it is shown, for the first time [3], that the number of propagating modes determines not only the conductivity, but the distinctive spatial distribution of the current-carrying electron states. The strong spacial quantization of the current-carrying states could be utilized in novel electronic δ-layer switches, where the number of propagating modes and their match/mis-match could be controlled by external electric fields, thus strongly affecting the current. In regular δ-layer conductors the particular distribution of current-carrying states directly affects their penetration depth into Si body and cap, which typically has a large concentration of impurities (see e.g. [12]). Thus, the control of the number of propagating modes may give an additional degree of control over the rate of impurity scattering. For $W > 10$ nm, the quantization effects gradually vanish and the conductivity tends to the infinitely-wide device values.

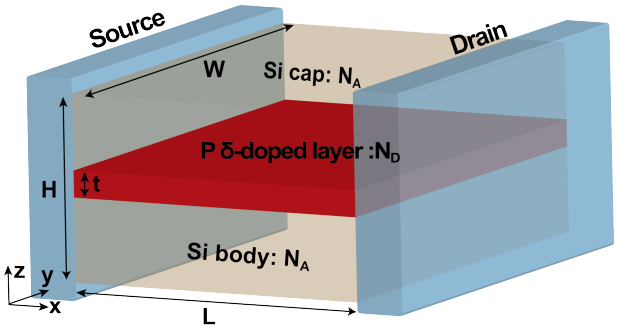

Figure 2: The Si:P δ-layer device is composed of a Si body, a very high P-doped layer and a Si cap. Open-system quantum-mechanical boundary conditions are applied at the source and drain regions; elastic scattering events are taken into account using the model discussed in [1].

2. Results and discussion

We have applied our open-system framework to investigate effects of size quantization in Si: P δ-layer systems on the conductivity. The device is shown in Fig. 2.

The corresponding dependence of the current on the device width W is shown in Fig. 3. The existence of the conduction steps due to each new propagating mode is well known experimentally since 1980's [13]. Here we report, however, that in highly-confined, highly-conductive δ-layer systems, the quantum number m, representing the number of propagating modes, determines not just the total current, but also the spatial distribution of the corresponding current-carrying electrons as also shown in Fig. 3. The total number of propagating modes m depends on the number of peaks in the density of states (DOS) and

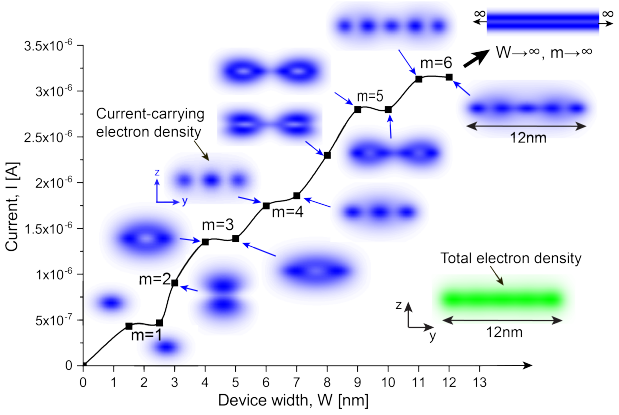

Figure 3: Propagation modes (m) for Si: P δ-layer systems. Current I vs device width W for δ-layer systems: the insets in blue color show the spatial distributions of current-carrying modes across a $y-z$ plane, indicating the corresponding number of propagating modes m; Inset in green color shows the total electron density that includes all (not just current-carrying) occupied electron states for a device width of $W = 12$ nm. For all calculations, $N_D = 1.0\times10^{14}$cm^{-2}, $N_A = 5.0\times10^{17}$ cm^{-3}, $t = 0.2$ nm and an applied voltage of 1 mV.

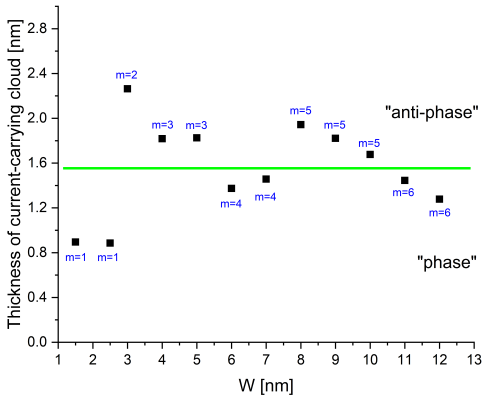

Figure 4: Computed average thickness of the *current-carrying electron cloud* in Si: P δ-layer systems vs device width W demonstrates that "phase" distributions ($m = 1,4,6,\ldots$) provide more compact placement of current-carrying electrons than "anti-phase" distributions ($m = 2,3,5,\ldots$). For all calculations, $N_D = 1.0\times10^{14}$cm^{-2}, $N_A = 5.0\times10^{17}$ cm^{-3}, $t = 0.2$ nm and an applied voltage of 1 mV.

is mainly determined by the three factors: 1) the δ-layer doping level N_D, 2) the the δ-layer doping thickness t and 3) the device width W.

The spatial distribution of the current-carrying electron states, $n_{curr.-carr.}(y,z)$, can be obtained by performing the energy integration of the local density of electron states (LDOS) weighted by the corresponding current spectrum $i(E)$ as: $n_{curr.-carr.}(y,z) = \int LDOS(y,z,E)i_e(E)dE/\int i_e(E)dE$. The spatial distribution of current-carrying electrons for the different device width values W is shown in Fig. 3 as insets in blue color, as well as the corresponding number of propagating mode m. Additionally, the total electron density is also included in the figure as an inset in green color, demonstrating only weak spatial quantization along the $y-$direction. However, the specific portion of electrons with energies close to the Fermi level, i.e. the current-carrying states, do exhibit a strong spatial quantization. Indeed, for $m = 1$ the propagating mode reaches the maximum concentration at the center of the structure, the mode the corresponds to $m = 2$ is "excited" into the further penetration along the confinement direction ($z-$axis), leaving the center relatively depopulated (in terms of the current-carrying states), the mode $m = 3$ is again "pushed out" of the center along both $z-$ and $y-$ axis. When $W \to \infty$, the number of propagation modes in $y-$direction becomes infinite $m \to \infty$ as expected. One can further note that the modes $m = 1$, and $m = 4,6$, etc. tend to form a regular "phase" distribution of the current-carrying states (i.e. the states distributed closer to the center of the δ-layer along z-axis), while the modes $m = 2$, and $m = 3,5$, etc. form "anti-phase" distributions (i.e. the states distributed further from the center of the δ-layer along z-axis) that have the maximum current being carried in the different regions of space, separated by a few nanometers. This is illustrated in Fig. 4 showing average current-carrying electron cloud thickness as a function of device W and, consequently, number of propagating modes m. As can be seen from this figure, "phase" current-carrying distributions ($m = 1,4,6,\ldots$) are located closer to the phosphorus δ-layer, while "anti-phase" current-carrying electrons ($m = 3,4,5,\ldots$) are always further away from the center of the δ-layer than "phase" distributions.

3. Conclusions

We employed an efficient computational open-system quantum-mechanical treatment to explore the conductive

properties of Si: P δ-layers, and the size quantization effects for sub-20 nm width δ-layers. We reported a strong spatial quantization of the current-carrying states for devices widths $W < 10$ nm, which could be utilized in novel electronic δ-layer switches. The number of propagating modes could be controlled by external electric fields, thus strongly affecting the current. For devices widths $W > 10$ nm, the quantization effects practically vanish and the conductivity tends to the infinitely-wide device values.

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