Strong Quantization of Current-carrying Electron States in $\delta$-layer Systems

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Abstract

We present an open-system quantum-mechanical real-space study of the conductive properties and size quantization in phosphorus $\delta$-layers systems, interesting for their beyond-Moore and quantum computing applications. Recently it has been demonstrated that an open-system quantum mechanical treatment provides a much more accurate match to ARPES measurements in highly-conductive, highly-confined systems than the traditional approaches (i.e. periodic or Dirichlet boundary conditions) and, furthermore, it allows accurate predictions of conductive properties of such systems from the first principles. Here we reveal that quantization effects are strong for device widths $W < 10$ nm, and we show, 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’s values.

Keywords: Si:P $\delta$-layer systems, quantum transport, Contact Block Reduction method

1. Introduction

Highly conductive $\delta$-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 [1], the conductive properties of such systems are expected to exhibit a strong influence of size quantization effects.

Recently it has been demonstrated in [2] that to extract accurately the conductive properties of highly-conductive, highly-confined systems, an open-system quantum-mechanical analysis is necessary, e.g. the Non-Equilibrium Green’s Function (NEGF) formalism. In this work we employ an efficient computational implementation of NEGF, which is called Contact Block Reduction (CBR) method [3, 4, 5, 6, 7], to investigate the conductive properties of Si: P $\delta$-layer systems and their size quantization. A flow-chart of the algorithm implemented in our CBR simulator is shown in Fig. [1]. For the charge self-consistent solution of the non-linear Poisson equation, we employ 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 Schrodinger equation with Dirichlet and open-system boundary conditions [3]), 2) the open-system predictor-corrector approach [5] and 3) the Anderson mixing scheme [7].

In this work we demonstrate that quantization effects are strong for device widths $W < 10$ nm, whereas, for $W > 10$ nm, the quantization effects gradually vanish and the conductivity tends to the infinitely-wide device’s values. Similarly, we also show, for the first time, that the number of propagating modes for narrow device widths determines not only the conductivity, but the distinctive spatial distribution of the current-carrying electron.
2. Results and discussion

We have applied our open-system framework to investigate the effects of size quantization in Si: P δ-layer systems on the conductivity at the cryogenic temperature of 4 K. The device is shown in Fig. 2, which is composed of a Si body, a very high P-doped layer and a Si cap. As discussed in [2], inelastic scattering is neglected since in Si:P δ-layer systems the phase-relaxation length $l_p$ is larger than the mean free path $l_m$ at low temperatures [9, 10]. However, we also note that all elastic scatterings, including electron-electron and electron-electric fields interactions, are taken into account in our method through the self-consistent Hartree + LDA exchange-correlation terms. Scattering on discrete charged impurities in δ-layer tunnel junctions was analysed in [11].

The corresponding dependence of the current (or, equivalently, the conductance) on the device width $W$ is shown in Fig. 3 taken from our work [8]. We first report that the size quantization effects are strong for device widths $W < 10\text{ nm}$, whereas, for $W > 10\text{ nm}$, the quantization effects gradually vanish and the conductivity tends to the infinitely-wide device’s values ($W \rightarrow \infty$) [8]. The existence of the conduction steps for narrow devices due to each new propagating mode is well known experimentally since 1980’s [12]. The total number of propagating modes $m$ depends on the number of peaks in the density of states (DOS) and is mainly determined by three factors: 1) the δ-layer doping level $N_D$, 2) the δ-layer doping thickness $t$, and 3) the device width $W$. 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.

The spatial distribution of the current-carrying electron states, $n_{\text{curr-carr}}(y, z)$, can be obtained by performing the energy integration of the local density of electron states (LDOS) weighted by the corresponding current spectrum $i(E)$ and normalized with the total current as: $n_{\text{curr-carr}}(y, z) = \int LDOS(y, z, E)i_{\text{curr}}(E)dE/\int i_{\text{curr}}(E)dE$. The spatial distribution of current-carrying electrons for different device widths $W$ is shown in Fig. 3.
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 and the current-carrying electron density (inset in blue color). Additionally, 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 that 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, and so on. When $W \to \infty$, the number of propagation modes in $y-$direction becomes infinite $m \to \infty$, as expected. Thus, 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 $\delta$-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 $\delta$-layer along $z$-axis). This is also illustrated in Fig. 4 showing the average current-carrying electron cloud thickness as a function of device width $W$ and the number of propagating modes $m$. As can be seen, "phase" current-carrying distributions ($m = 1, 4, 6, \ldots$) are located closer to the phosphorus $\delta$-layer, while "anti-phase" current-carrying electrons ($m = 3, 4, 5, \ldots$) are further away from the center of the $\delta$-layer than "phase" distributions.

Finally, we also note that this strong spacial quantization of the current-carrying states for narrow device widths could be utilized in novel electronic $\delta$-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. Additionally, in regular $\delta$-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. [13]). Thus, the control of the number of propagating modes may give an additional degree of control over the rate of impurity scattering.
3. Conclusions

We employed an efficient computational open-system quantum-mechanical treatment to explore the conductive properties of Si: P δ-layer systems and their size quantization effects for sub-20 nm width δ-layers. We reported a strong spatial quantization of the current-carrying states for device widths $W < 10$ nm, which could be utilized in novel electronic δ-layer switches. The number of propagating modes $m$ determines not just the total current, but also the spatial distribution of the corresponding current-carrying electrons. For device widths $W > 10$ nm, the quantization effects practically vanish and the conductivity tends to the infinitely-wide device’s values.

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