Quantum Transport Framework for Highly Conductive δ-layer Systems

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The need for alternative beyond-Moore computing systems has raised a particular interest in δ-layer systems, which consist of a very highly doped monolayer of dopants in an intrinsic semiconductor. These systems have shown promising applications due to their high current density. Several approaches have been used to investigate such systems. However, these approaches are mainly based on periodic boundary conditions along the propagation direction, i.e. the in-plane direction. Therefore, they are mainly limited to investigate equilibrium properties, and additional approximations are required to extract the conductive properties.

In this work, we propose a new open-system quantum transport (QT) framework, based on the Non-Equilibrium Green Function (NEGF) and the effective mass theory, which allow us a direct way to investigate the conductive properties of δ-layer systems. Our QT framework requires a repeated solution of the effective mass Schrödinger equation and the non-linear Poisson equation [1-4] (Fig. 1). For an efficient implementation of the NEGF formalism, we utilized the Contact Block Reduction (CBR) method [1,2]; and, for the charge self-consistent solution of the non-linear Poisson equation, we employed a combination of the predictor-corrector approach and Anderson mixing scheme [3,4].

We have applied this QT framework to study the conductive band structure and the corresponding conductive properties for Si:P δ-layer wires (Fig. 2). Our simulations reveal new physics insights. Firstly, our LDOS analysis predicts a peculiar quantized structure of the conductive sub-bands (Fig. 3), as well as it shows that the free electrons are spatially separated in layers with different average kinetic energies (Fig. 3). Secondly, the number of existing conductive sub-bands is determined by the thickness and sheet doping density of the δ-layer. Finally, as a result of this quantized sub-band structure, we predict: 1) a non-linear dependence of the electron cloud confinement on the δ-layer doping profile (Fig. 4); 2) an increase of the sheet resistivity for sharper δ-layer doping profiles (Fig. 5).

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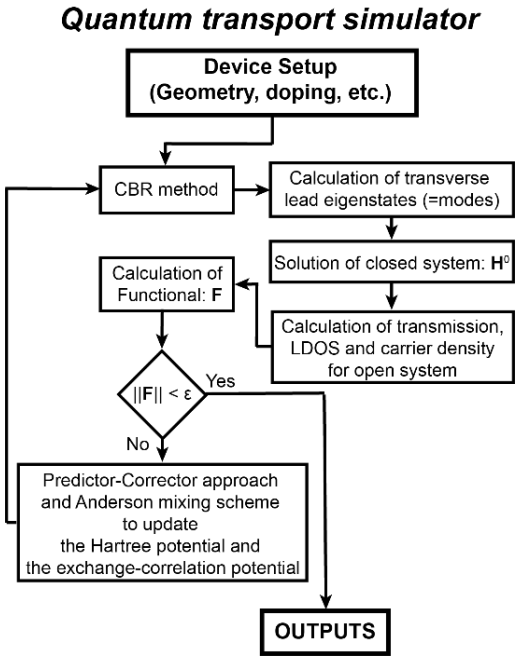

Fig. 1: A simplified flow chart of the self-consistent Quantum Transport method to solve the effective mass Schrödinger equation and the non-linear Poisson equation. ε is the non-linear Poisson residuum tolerance.

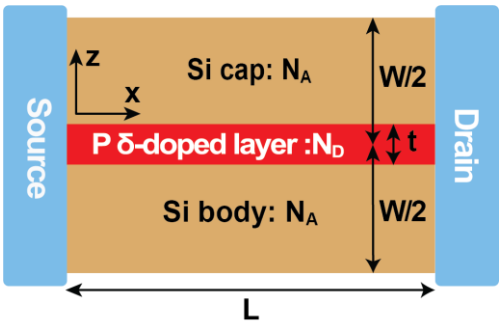

Fig. 2: Schematic model of the Si:P δ-layer system. It is composed of a Si body, a very high P-doped layer, and a Si cap. The conductor channel is in contact with two semi-infinite leads, the source, and drain, respectively.

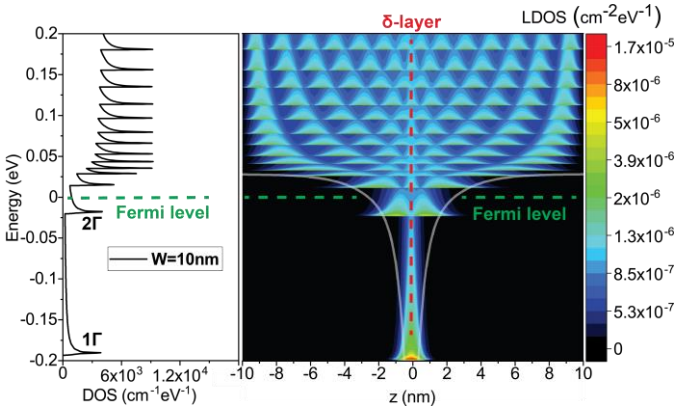

Fig. 3: Right panel: LDOS(z,E) of a Si: P δ-layer wire (W=20nm and an acceptor density of 10^{17} cm^{-3}). Left panel: corresponding total DOS of the system.

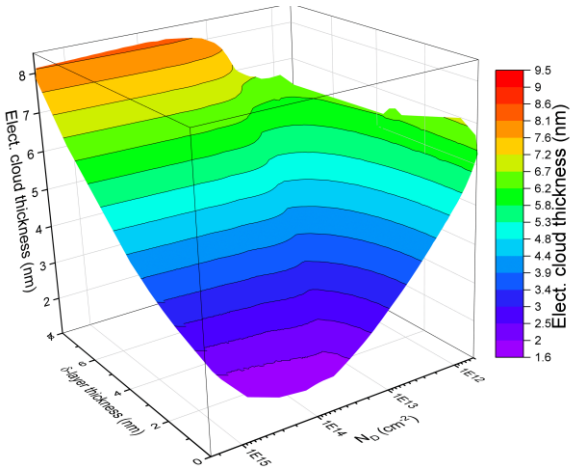

Fig. 4: Effective electron cloud thickness around the δ-layer plane as a function of the δ-layer thickness and the sheet doping density N_D.

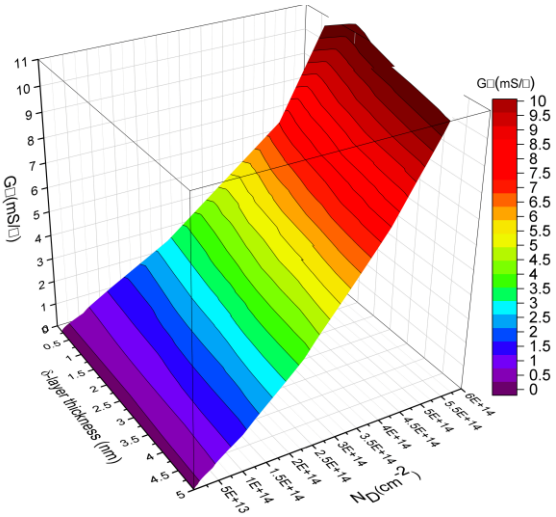

Fig. 5. Sheet electrical conductance for Si: P δ-layer wire in function of the δ-layer thickness and doping density.

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