Impurity Potential Induced Resonances in Doped Si Nanowire: Non-Equilibrium Green's Functions Simulations

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A coherent transport of electrons through a uniformly doped silicon quantum wire in the presence of one impurity in the channel is studied using fully 3D Non-Equilibrium Greens Functions technique. The potential of the single impurity, assumed to be attractive (a donor), is self-consistently calculated via Poisson equation coupled with Schrdinger equation in the effective mass approximation. The effects of the screening on the donor and of the polarization at the Si/SiO2 interface are included in a non-perturbative way (in the Hartrees approximation). The transmission shows different types of resonances (Breit-Wigner and Fano types) from the quasi-bound states of the impurity when compared to the impurity free wire. The study has significant relevance to mesoscopic wires and nanowire transistors.