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Full band quantum transport using mixed supercell and envelop function method[1] JINGTIAN FANG, WILLIAM VANDENBERGHE, MASSIMO FISCHETTI, The University of Texas at Dallas — We study one-dimensional quantum transport in field-effect transistors with different channel materials, such as silicon nanowires, graphene nanoribbons, and carbon nanotubes. The normal (real) band structure and the complex band structure are calculated using the local empirical pseudopotential method. We employ the supercell approach to treat the two-dimensional quantum confinement and the envelop wavefunction approximation to deal with the open-boundary-condition transport problem. The proper open boundary conditions for atomically homogeneous systems along the transport direction are derived using the complex band structure of the contacts. The computational cost for solving the real-space quantum transport equation strongly increases when large cutoff energies are used and more realistic devices are simulated. We use a parallel computation technique to model devices with a length of 10 nm or larger. A sparse matrix solver enables the efficient solution of the transport equations as well. We present the electron density and potential profile in the device along the transport direction. The current-voltage characteristics of the device show that the current is almost linearly increasing when low biases are applied.

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