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Coarse-grained quantum transport simulation for analyzing leakage-mobility antagonism in GNRFET MASAKATSU ITO, SHINTARO SATO, NAOKI YOKOYAMA, National Institute of Advanced Industrial Science and Technology (AIST), CHRISTIAN JOACHIM, Centre d'Elaboration des Matériaux et d'Etudes Structurales (CEMES-CNRS) & MANA Satellite, GREEN NANOELECTRONICS CENTER TEAM, CEMES-CNRS & MANA SATELLITE COLLABORATION — Since it became clear that graphene transistors based on the classical MOSFET principle suffer from serious performance problems, researchers have explored new graphene device design using quantum transport simulations. A first-principle quantum transport simulation, however, still takes unaffordable computational cost to deal with a realistic size of graphene transistor ($> 10^4$ atoms). This motivated us to import ESQC (elastic scattering quantum chemistry) technique from the research field of molecular electronics and to develop its coarse-grained version. To eliminate the atomic scale details, we reformulated ESQC technique using the continuum limit description of graphene charge carriers, which is given by the massless Dirac equation. Since the potential function in this Dirac equation is electrostatic potential distribution, it can be obtained from Poisson equation with the boundary conditions of gate voltages in a self-consistent manner. We are now applying this coarse-grained quantum transport simulation to GNRFETs (graphene nanoribbon field effect transistors) for resolving the mobility-leakage antagonism, where opening a bandgap in a graphene channel improves its switching ability but at the same time deteriorates the electron channel mobility.

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