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GPU Accelerated Quantum Transport Modelling of Realistic Large Cross-Section Silicon Nanobeams MOHAMMED HARB, HONG GUO, McGill University — Understanding the quantum transport properties of silicon nano-beams or -wires is important for many practical applications. But for nanobeams with a cross section larger than 10 nm square or so, typical transport modelling techniques based on Green's functions and atomistic DFT Hamiltonians become very computationally demanding. The computational burden becomes even greater when electron scattering with phonons is included. In this work we report hardware acceleration of the computational algorithm using a cluster of CPUs and GPUs working together in a heterogenous computing scheme. The GPU accelerated transport technique is implemented for atomistic tight-binding Hamiltonian within the non-equilibrium Green's function formalism. As examples, we calculate charge transport properties of realistic large cross-section Si nanobeams with several defect configurations, and report how local density of states can be significantly perturbed by the presence of the atomic impurity.

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