Simulation of Silicon Nanodevices at Cryogenic Temperatures for Quantum Computing

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Abstract

Electronic devices operating at cryogenic temperatures are critical for a wide variety of applications including quantum computing, space, medicine and fundamental research [1]. The design of these devices requires accurate physical modeling of the electric fields, currents, conduction band energies and electron densities at low temperature. While there are several commercial modeling platforms for performing these calculations accurately, the COMSOL Multiphysics Software offers the combined advantage of flexibility and capability to solve for several independent physical equations in a self-consistent manner. However, modeling semiconductor devices at cryogenic temperature using iterative methods poses numerical convergence issues because the electron density scales exponentially with temperature. This leads to intermediate solutions that have sharp discontinuities in the fields. We report on methods to ease convergence and thereby extend modeling to the case of silicon based devices at low temperature using the COMSOL Semiconductor module. We illustrate this with an example of a realistic 3-D prototype nanodevice that can be used to read out the state of a quantum bit (qubit) in a silicon quantum computer [2]. With proper choices of the finite-element solver, equations, initial values for the electron density, auxiliary parametric sweeps and an efficient mesh, we achieve convergence down to ∼15 Kelvin. We then simulate the required conduction band energies, electric fields and qubit positions for readout in the nanostructure [3]. We also provide a systematic analysis of the above parameters with temperature, and use them to establish the accuracy of our simulations. Our results for this specific nanostructure directly fits into a broader context of developing a computational workflow to accurately design silicon qubit devices for quantum computing [4]. The methods and parameters employed in this work can also be leveraged to tackle convergence issues for a variety of semiconductor devices operating at low temperature.

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[3] F. A. Mohiyaddin et. al., Noninvasive Spatial Metrology of Single-Atom Devices, Nano Letters, 13, 5, 1903-1909, April 2013.
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Figures used in the abstract

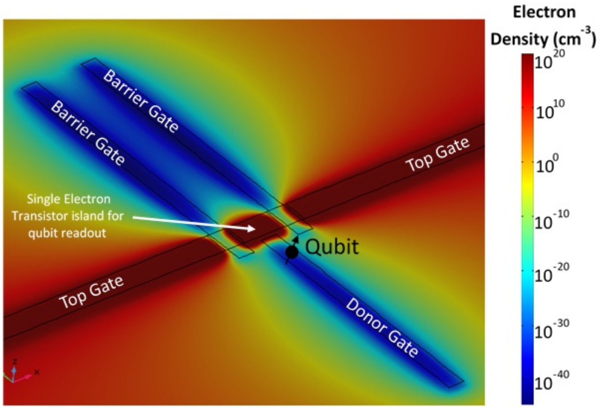

Figure 1: Electron density in a nanostructure where a quantum bit (qubit) is read out