Multi-subband Monte Carlo Simulations of Hole Mobility in Silicon Nanowire FETs

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INTRODUCTION

Motivation: Silicon Nanowire (Si NW) FETs have gained attention due to the enhanced channel control [1]. While parabolic effective mass model has been widely used to model transport behaviors [2], it not only loses accuracy in predicting state-quantization in sub-nm structures [3], but also fails to model the valence sub-bands needed to explain the hole physics [4]. Quantum transport in sub-nm FETs can be calculated via non-equilbrium green's function method [5]. Scattering-involved transport problems in multi-subband systems, however, need too much computing load [6].

Objective and Impact: The hole mobility in Si NWs is discussed via multi-subband Monte Carlo method coupled to 2-D Schrödinger-Poisson simulations. We not only explore the mobility pattern against the channel inversion charge density, size, and transport direction, but also predict the main scattering mechanism that degrades the mobility. Previous works are limited to the electron mobility study [7], focus on the acoustic phonon scattering only [8], or miss self-consistent calculations and a connection to experimentally known result [9].

METHODOLOGY

Electronic Structure: The low-field transport is simulated assuming gate-all-around intrinsic long channels with a 1nm thick SiO_2 layer and a periodic boundary condition along the transport direction (Fig. 1(a)). Ignoring the spin-orbit coupling, channels are represented with 3-band $k{\cdot}p$ model [4] focusing on valence band structures.

Electrostatics and Mobility: Starting from self-consistently determined channel potential and subband profiles, the hole mobility is calculated with 1-D Boltzmann transport equation coupled to Monte Carlo method (Fig. 1(b)). Acoustic, non-polar optical phonon and surface roughness scattering (SRS) are considered where the impurity coulomb scattering is ignored assuming intrinsic channels.

Simulation Case: [100] and [110] transport direction are considered at T=300K where the gate lead and channel are assumed to have the same work function. For each direction, 5 cross-section sizes (3nm to 10nm) are simulated with a total of 11 bias points per each size (0.0V to -1.0V).

RESULT AND DISCUSSION

Low-field Mobility: Fig. 2 shows the hole mobility plotted against the inversion charge density instead of the gate-bias for clear discussions, where the mobility decreases as a channel has a smaller cross-section and is inverted more strongly. The result here is reasonable as the phonon scattering rate increases for a stronger structural confinement [8], and the SRS rate also increases with an increasing charge density and at a smaller cross-section size.

If the channel is not strongly inverted, [110] channels show a slightly higher mobility at a 10nm cross-section while [100] channels show a higher mobility at cross-sections ≤ 6nm. But, when strongly inverted, the mobility is rapidly degraded in both cases (we will be back to this issue). As the cross-section size increases, the mobility reaches the intrinsic Si bulk value (~500 (cm^2/V/sec)) regardless of transport directions, which becomes the strong evidence validating this work.

Scattering Mechanism: The mobility pattern with respect to transport directions can be easily understood by looking into the mobility limited by the phonon (acoustic+optical) scattering (PH) and SRS (Fig. 3). For a 10nm cross-section channel that is not strongly inverted, the PH-limited mobility is smaller than, or comparable to SRS-limited one, and PH thus affects the hole mobility as similarly as, or a bit more than SRS does. As the PH-limited mobility is higher in [110] channels, the hole mobility in [110] channels is also slightly higher than, or comparable to the mobility in [100] channels.

If the cross-section is downscaled to a few nm size or the channel is strongly inverted, the SRS-limited mobility is degraded more rapidly than the PH-limited one, dominating the hole mobility. As the SRS-limited mobility becomes larger in [100] channels, so does the hole mobility although the difference is not quite discernable as the mobility is already too small in both channels.

CONCLUSIONS

By simulating the low-field hole transport in Si NWs, we found that SRS becomes the dominant scattering mechanism, by which the hole mobility is significantly degraded when the channel cross-section is in a few nm size or strongly inverted.

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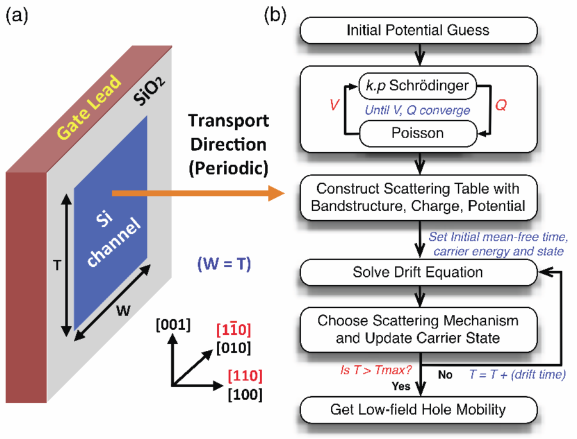

Fig. 1. (a) Illustration of the gate-all-around Si NW geometry (b) A flow chart of multi-subband Monte Carlo approach coupled to Schrödinger-Poisson simulations.

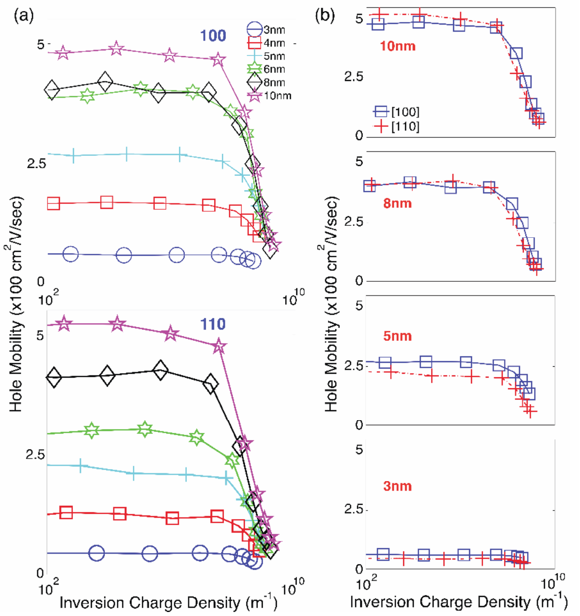

Fig. 2. (a) Dependence of the hole mobility on the inversion charge density, cross-section size, and transport direction. (b) The hole mobility at selected channel cross-section sizes. Unless the channel is strongly inverted, the mobility is higher in [110] channels at 10nm cross-section while [100] channels show a larger mobility as the cross-section is downscaled.

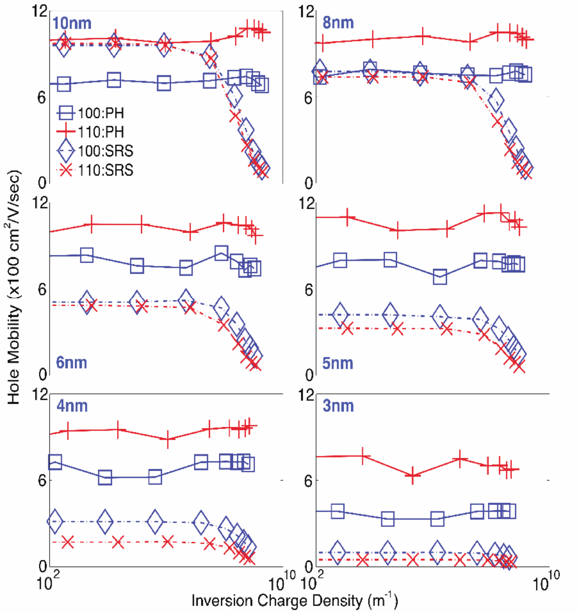

Fig. 3. The mobility limited by PH and SRS. When the NW channel has a large cross-section and is not strongly inverted, PH affects the hole mobility as similarly as or more strongly than SRS does. If the cross-section is smaller than 6nm, or the channel is strongly inverted, the SRS-limited mobility becomes smaller than the PH-limited one, dominating the hole mobility.