Thermoelectric properties of gated Si nanowires

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INTRODUCTION

The thermoelectric (TE) performance of materials is determined by the figure of merit $ZT=\sigma S^2/\kappa$, where σ denotes the electrical conductivity, S the Seebeck coefficient and κ the thermal conductivity. Large improvements in ZT have recently been reported in nanoscale materials due to drastic reduction in κ. Despite this improvement, however, ZT still remains too low for allowing large scale TE deployment, mainly because the power factor (σS^2) has not been improved so far. A possible way to improve σS^2 is the use of gating rather than doping to achieve the required high charge densities [1]. This removes the strongest scattering mechanism that hinders carrier transport and yields higher conductivity. In this work, we compute the TE power factor in gated Si nanowires (NWs) and compare it to the power factor of doped NWs. We show that although gated structures suffer from reduced Seebeck coefficient, the power factor can be improved by ~5x.

METHOD AND DISCUSSION

We use the $sp^3d^5s^*$ tight-binding model for the electronic structure, self-consistently coupled to the 2D Poisson equation [2], as shown in Fig. 1. Upon convergence, the mobility is extracted using linearized Boltzmann transport theory. We consider acoustic phonons, optical phonons, surface roughness scattering, and ionized impurity scattering (for the ungated structures) [3]. We consider [110] p-type NWs of 12nm in diameter.

Figure 2 shows the carrier mobility versus density for two different device cases: i) the gated channel, considering phonon (red-solid-dot line) and surface roughness (red-dashed-dot line) scattering, and ii) the doped channel, considering phonons, surface roughness, and ionized impurity scattering (black-solid line). It can be observed that the mobility of the gated channel is largely increased compared to the mobility of the doped channel. In the accumulation layer formed, surface roughness scattering is not strong enough to significantly affect mobility even up to hole concentrations $p{\sim}5x10^{19}/cm^3$. Especially around $p{\sim}10^{19}/cm^3$, the carrier concentration most relevant for TEs, the mobility in the gated structure shows a large additional increase, related to modifications of the valence bandstructure upon gating. This is depicted in Fig. 3. The electronic structure at high gate bias (Fig. 3b) acquires a larger curvature compared to the equilibrium bandstructure shown in Fig. 3a (see Ref. [2] for details). The larger curvature provides higher carrier velocities, and thus, higher carrier mobility. The Seebeck coefficient shown in Fig. 4, on the other hand, suffers in the gated structures compared to the doped channels, although surface roughness scattering provides a small increase. The improvement in mobility, however, outperforms the reduction in the Seebeck coefficient. The TE power factor shown in Fig. 5, is thus greatly enhanced in the gated structures (red-solid-dot line) compared to doped channels (black-solid). An improvement of the order of ~5x is observed, peaking at $p{\sim}10^{19}/cm^3$. Note that this improvement is reduced as the NW diameter increases, but we estimate that some improvement is retained for NWs with diameters even up to 30nm.

CONCLUSION

Using the $sp^3d^5s^*$ tight-binding model, coupled to thelinearized Boltzmann equation and the Poisson equation, we calculate the thermoelectric power factor of p-type [110] Si nanowires. We show that gated Si NWs offer the possibility of improved thermoelectric power factors by up to ~5x compared to doped NW channels due to the high phonon-limited hole mobility and bandstructure modifications under electrostatic confinement.

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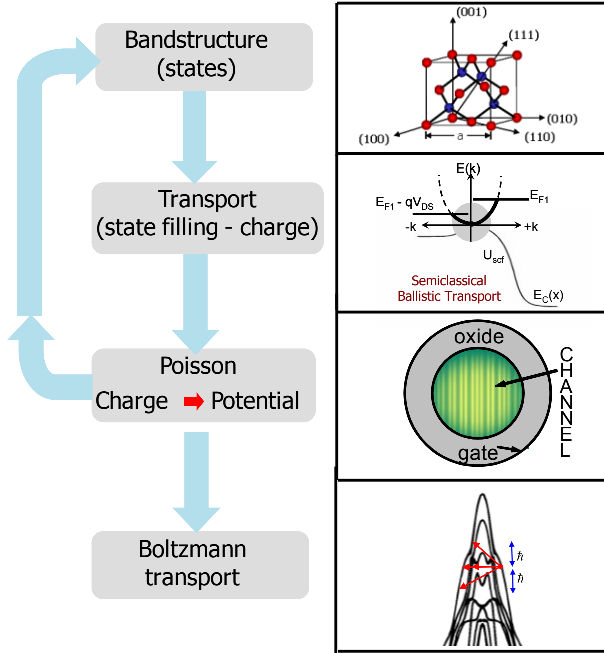

Fig. 1. Simulation procedure. (a) The NW bandstructure is calculated using the $sp^3d^5s^*$ TB model. (b) A semiclassical model is used to calculate the charge distribution in the gated NW. (c) The charge is self-consistently coupled to a 2D Poisson equation for the electrostatic potential in the cross section of the wire. The oxide is assumed to be SiO_2 of thickness t_{ox}=1.1nm (d) Upon convergence (and at V_D=0V), Boltzmann transport theory, including all relevant scattering mechanisms, is used for mobility calculations.

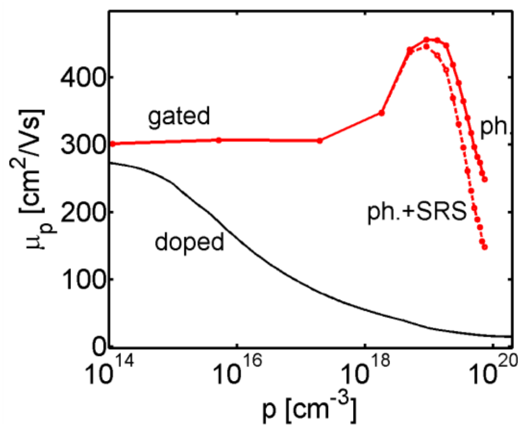

Fig. 2. Mobility versus density. Showing results for gated NWs (red-dot) under i) phonon-limited (solid), and ii) phonon-SRS-limited transport (dashed), and doped NW (black-solid).

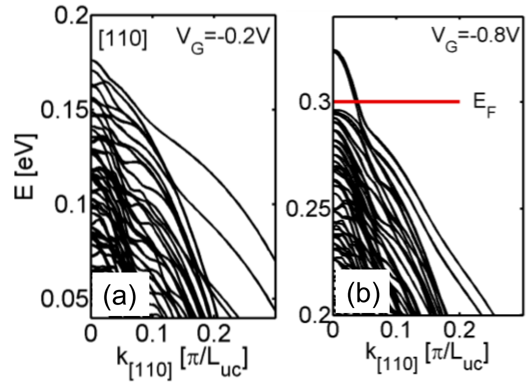

Fig. 3. Dispersions of the gated NW for different gate biases. (a) V_G=-0.2V (equilibrium / flat band), (b) V_G=-0.8V. The position of the Fermi level in (b) is indicated by the red line.

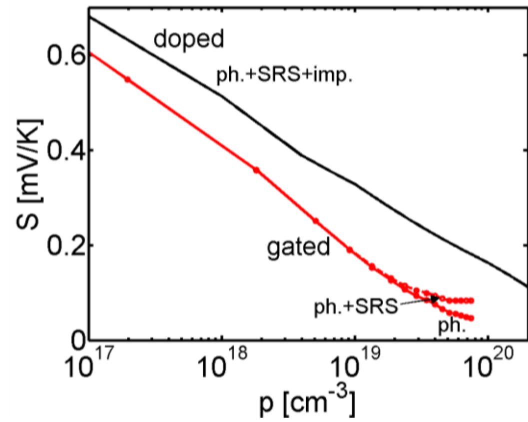

Fig. 4. Seebeck coefficient versus density. Showing results for gated NWs (red-dot) under i) phonon-limited (solid), and ii) phonon-SRS-limited transport (dashed), and doped NW (black-solid).

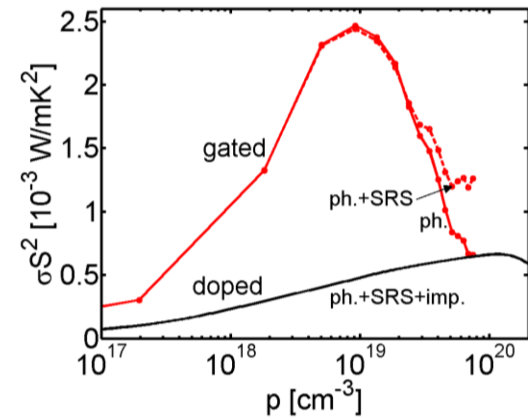

Fig. 5. Power factor versus density. Showing results for gated NWs (red-dot) under i) phonon-limited (solid), and ii) phonon-SRS-limited transport (dashed), and doped NW (black-solid).