Confinement-Induced Mobility Increase in p-type [110] and [111] Silicon Nanowires

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1. Abstract

The $sp^3d^5s^*$-spin-orbit-coupled (SO) atomistic tight-binding (TB) model is coupled to Boltzmann transport formalism for calculation of the low-field mobility in Si nanowires (NWs). We show that the phonon limited mobility of p-type NWs in the [110] and [111] transport orientations largely increases by more than 7X as the diameter is scaled from D=12nm down to D=3nm. This effect is attributed to dispersion modifications due to confinement that largely improve the carrier velocities and reduce scattering rates in these type of NWs.

2. Approach

Silicon NWs have recently attracted significant attention as candidates for high performance transistor channels. NW devices with channel lengths down to L_G=15nm and diameters down to D=3nm have already been demonstrated [1, 2].

Low-dimensional materials offer the capability of improved performance due to additional degrees of freedom in engineering their properties: i) the cross section size, ii) the transport orientation, iii) the orientation of the confining surfaces.

We calculate the phonon-limited mobility of p-type Si NWs using the $sp^3d^5s^*$-SO TB model for the electronic structure [3], and Boltzmann theory for transport [4, 5], for NWs up to 12nm in diameter (~5500 atoms in the unit cell). The conductivity is evaluated from:

$$\sigma = q_0{}^2 \int_{E_0}^{\infty} dE \left(-\frac{\partial f_0}{\partial E} \right) \Xi(E) \qquad (1),$$

where $\Xi(E)$ is defined as:

$$\Xi(E) = \sum_{k_x, n} v_n{}^2(k_x)\, \tau_n(k_x)\, \delta\left(E - E_n(k_x)\right) \qquad (2).$$

Here $v_n(k_x)$ is the bandstructure velocity and $\tau_n(k_x)$ is the momentum relaxation time for a hole with momentum k_x in subband n. The mobility is defined as:

$$\mu_p = \frac{\sigma}{q_0 p} \qquad (3),$$

where p is the hole concentration in the channel.

3. Results

Figure 1 shows the heavy-hole energy surface of bulk silicon. Confinement in the [110] direction will produce channels with light subbands picked alone the 45° lines in the figure. In a (110) ultra-thin-body (UTB) channel, this will result in lighter subbands in the [110] direction as the confinement increases. This is shown in Fig. 2a and 2b for this (110) UTB channel for body thicknesses W=3nm and W=15nm, respectively. In a NW, this effect will also result in lighter subbands with confinement, as shown in Fig. 3a and 3b for cylindrical [110] p-type NWs of D=3nm and D=12nm respectively.

The increase in the dispersions' curvature with confinement will result in increased carrier velocities and conductivity in the NWs. Figure 4 shows the carrier velocity in the p-type [110] (triangle-red) and [111] (circle-green) NWs. As the diameter decreases from D=12nm down to D=3nm, a ~2X increase in the velocity is observed. Figure 5 shows the conductivity in these NWs as a function of the carrier concentration for D=12nm (dotted) and D=3nm (solid). The conductivity largely increases for smaller diameters. This increase reflects in the mobility of the NWs as a function of the diameter as shown in Fig. 6. Here the mobility increases by 9X and 7X for the [110] and [111] NWs respectively as the diameter scales. We mention that only phonon scattering is considered in the calculations. Surface roughness scattering can change the results for very small diameters, but even so, mobility improvements with confinement can still be achieved [5].

4. Conclusions

The $sp^3d^5s^*$-SO atomistic tight-binding model is coupled to linearized Boltzmann transport for the calculation of mobility in silicon NWs. We show that the phonon-limited low-field mobility in p-type [110] and [111] NWs increases by 9X and 7X, respectively, as the diameter is reduced from D=12nm down to D=3nm.

References

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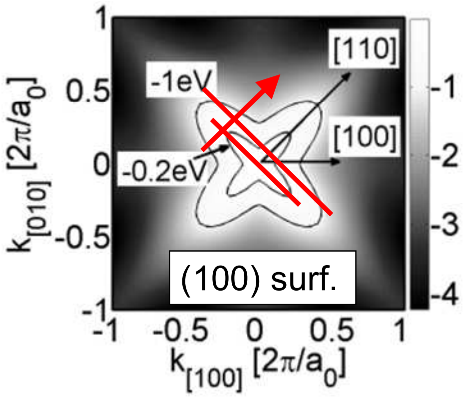

Fig.1: *The Si bulk (100) energy surface. The 45° inclined lines show the relevant energy regions for devices with physical surface confinement along the direction of the red arrow.*

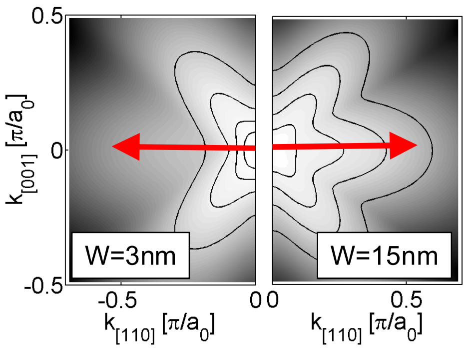

Fig.2: *The energy surfaces of (110) UTB layers for different thicknesses (W).Left:W=3nm. Right: W=15nm.The subbands are lighter in [110] (arrow) for the thinner body channel (the energy contours point towards the center).*

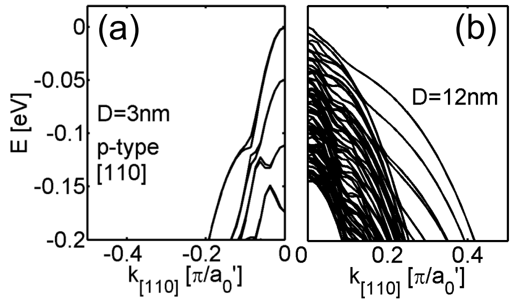

Fig.2: *Dispersions of p-type [110] NWs of diameters D=3nm (left) and D=12nm (right).*

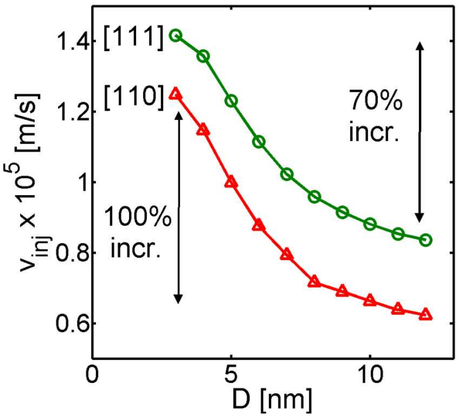

Fig.2: *The carrier velocities of p-type NWs in [110] (triangle-red) and [111] (circle-green) transport orientations vs. diameter under non-degenerate conditions.*

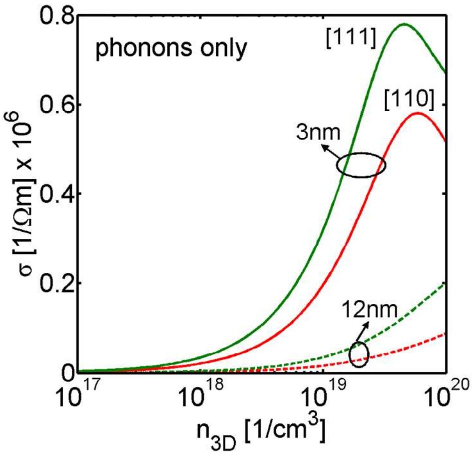

Fig.2: *The conductivity of p-type NWs in [110] (red) and [111] (green) transport orientations vs. the carrier concentration. Solid lines: D=3nm. Dashed lines: D=12nm.*

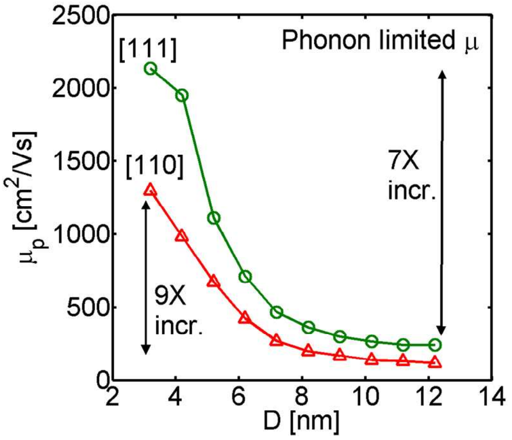

Fig.2: *Phonon-limited mobility for p-type NWs in [110] (triangle-red) and [111] (circle-green) transport orientations as a function of the NWs' diameter. Large increases are observed with diameter scaling.*