Impact of the Phonon Confinement and Geometry on the Mobility of Si-Nanowires

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INTRODUCTION

The continuous reduction of device dimensions imposed by the Moore's Law has focused the attention on non-planar devices such as Trigate MOSFETs or Gate-All-Around Silicon Nanowires (NWs). Therefore, the study of the transport properties in 2D-confined nanowires with sizes ranging in a few nanometers is a research field of high interest [1], [2]. As the size of the devices decreases, the modification in the acoustic phonon spectrum becomes more pronounced, making mandatory the inclusion of acoustic phonon confinement in the mobility calculation [3], [4]. In this work we assess the influence of the phonon confinement on the mobility of Si NWs with different sizes and geometries.

RESULTS

To study the confined phonon-limited mobility in arbitrarily shaped NWs we have simulated devices like those in Fig. 1, with SiO_2/HfO_2 as gate insulator (T_{SiO_2}=0.5nm, T_{HfO_2}=2nm), midgap metal gate, undoped body and different sizes with the standard orientation ([100]). For NWs with W_{Si} larger than 5nm, the effective mass approach provides accurate enough results [5]. The Kubo-Greenwood formula and the momentum relaxation time approach [2] have been used to estimate the phonon-limited low-field mobility which is evaluated utilizing the confined acoustic phonons under freestanding (FSBC) and clamped surface (CSBC) boundary conditions (applied at the Si/SiO_2 interface) as well as bulk acoustic phonons (NC). In order to calculate the confined phonon spectrum we solve the elastic wave equation [6], [7]

$$\rho\omega^2 u_i + \sum_l \frac{\partial \sigma_{li}}{\partial x_l} = 0 \qquad (1)$$

where ρ is the material density, ω is the angular frequency, u_i is the i-th component of the displacement vector, σ_{li} is the stress tensor and x_l can be the x, y or z coordinate. For the FSBC we have used the xyz algorithm proposed in [7] whereas for the CSBCs, we have selected a set of basis functions that vanish at the Si/SiO_2 interface to satisfy the boundary conditions ($u_i|_S$=0). Both methods can be employed regardless the geometry of the device.

Figure 2 shows the phonon dispersion for a W_{Si}=5nm square NW using the FSBC and the CSBC. Only the lowest phononic subbands are depicted. As can be seen, the use of CSBC makes the nearly linear phonon mode disappear provoking an increase in the carrier mobility as can be noticed in Fig. 3 where the phonon-limited mobility has been depicted for the same device when FSBC, CSBC and NC phonons are taken into account.

Figure 4 depicts the phonon-limited mobility of square devices with different sizes at $N_i = 5 \times 10^6 cm^{-1}$. As can be seen, the smaller the device, the bigger the effect of the different boundary conditions. As expected, in the limit of a large size, the FSBC and the CSBC curves approach the NC one.

Finally we have assessed the effect of the geometry on the mobility through the simulation of NWs with different percentage of curvature in their corners. Figure 5 depicts the mobility calculated when FSBC, CSBC and NC phonons are taken into account for a W_{Si}=5nm device with a percentage of curvature of 50% (left) and 100% (right). When compared to Fig. 3 (square NW), we have observed a decrease in the phonon-limited mobility as the rounding of the corners increases regardless of the phonon description employed.

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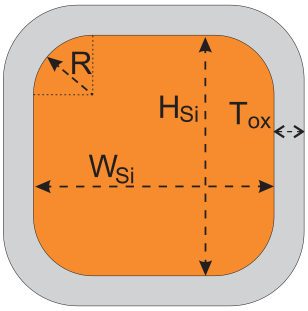

Fig. 1. Geometry of the devices under study. W_{Si} and H_{Si} are the device width and height, $\mathrm{T_{ox}}$ is the insulator thickness and R determines the percentage of curvature of the device as $100 \cdot 2R/W_{\mathrm{Si}}$.

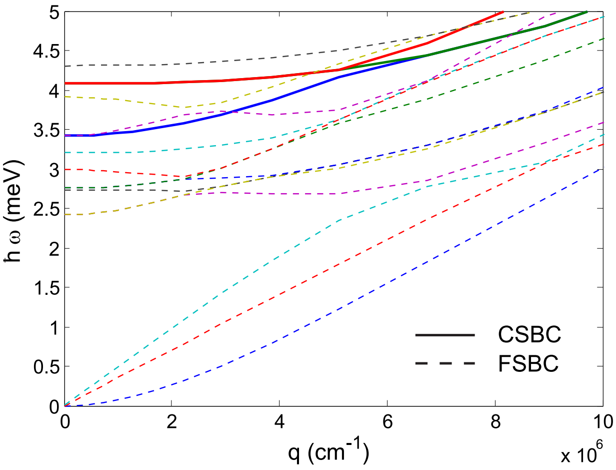

Fig. 2. Phonon dispersion relation for a $\mathrm{W_{Si}}$=5nm square (R=0) NW when FSBC (dashed lines) and CSBC (solid lines) are considered.

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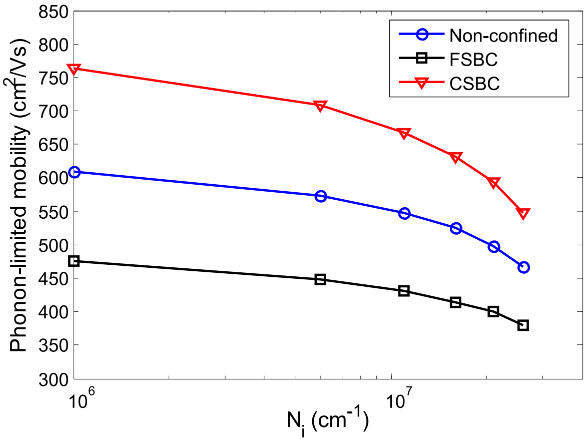

Fig. 3. Phonon-limited mobility vs. $\mathrm{N_i}$ for a $\mathrm{W_{Si}}$=5nm square (R=0) NW when NC phonons (circles), FSBC (squares) and CSBC (triangles) are considered.

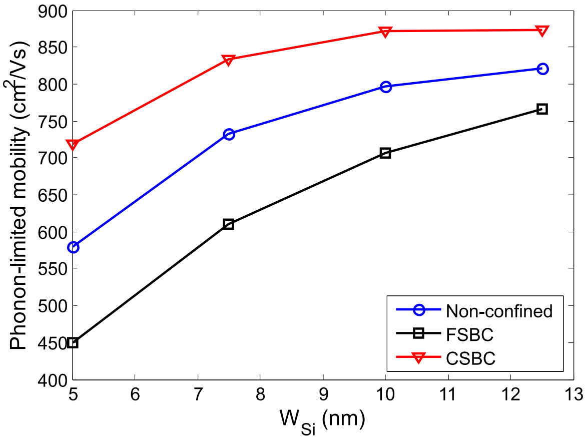

Fig. 4. Phonon-limited mobility vs. size for square (R=0) NWs at $\mathrm{N_i} = 5 \times 10^6 \mathrm{cm}^{-1}$ when NC phonons (circles), FSBC (squares) and CSBC (triangles) are considered.

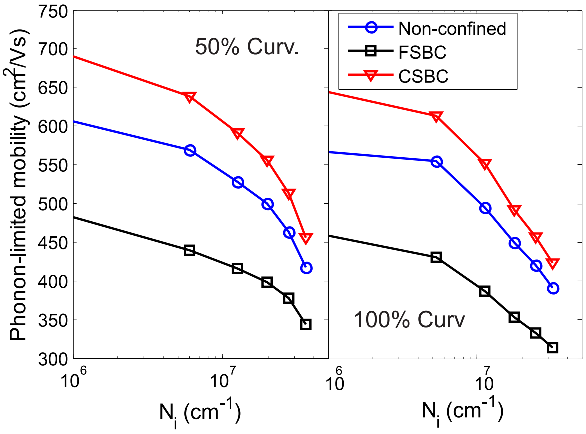

Fig. 5. Phonon-limited mobility vs. $\mathrm{N_i}$ for $\mathrm{W_{Si}}$=5nm NWs with 50% (left) and 100% (right) percentage of curvature when NC phonons (circles), FSBC (squares) and CSBC (triangles) are considered.