Influence of strains on the electron and hole mobility in silicon nanowires

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The use of mechanical strains has become an attractive solution to improve the electrical performances of silicon devices. Silicon nanowires (Si NWs) can actually withstand large non-intentional strains due to oxidation or other processing steps, and can easily be stretched on purpose. In this talk, we investigate the phonon-limited electron and hole mobilities of strained Si NWs with a fully atomistic semi-empirical approach. We show that the mobility can be enhanced or reduced by a factor > 2 for moderate strain, and discuss the physics behind these trends.

METHOD

The phonon-limited mobility of the Si NWs is computed in a fully atomistic semi-classical framework. The electronic structure of the Si NWs is computed with the $sp^3d^5s^*$ tight-binding (TB) model of Ref. [1], and the phonons with the valence force field (VFF) model of Ref. [2]. The electron-phonon scattering rates are then calculated from the derivatives of the TB hamiltonian with respect to the atomic positions. The linearized Boltzmann equation is finally solved exactly for the low-field mobility. Details can be found in Ref. [3].

In the following, the Si NWs are stretched along their axis, and the atomic positions within the strained unit cell are relaxed with the VFF model.

RESULTS

The electron mobility in a $\langle 110 \rangle$ Si NW with diameter $d = 8$ nm is plotted as a function of the axial strain $\varepsilon_{\parallel}$ in Fig. 1. It can vary by a factor as large as $\simeq 2$ in a moderate strain range $\varepsilon_{\parallel} \in [-1\%, 1\%]$.

These trends result from band structure effects. Tensile strain lowers the ground-state, light Δ_z valleys at Γ with respect to the heavier $\Delta_{x,y}$ valleys near the zone edge (see Figs. 2, 3, and 4). This increases the proportion of fast Δ_z electrons, suppresses inter-valley scattering, and therefore enhances the mobility. Conversely, compressive strain reduces the splitting between the Δ_z and $\Delta_{x,y}$ valleys. The latter actually become the ground state valleys for strains $\varepsilon_{\parallel} < -0.25\%$. Notice the non-linear behavior of the Δ_z valleys on Fig. 4, and the decrease of the mobility at large $\varepsilon_{\parallel} > 1\%$, which are both due to the effects of the Ξ'_u conduction band shear deformation potential.

The hole mobility in a $\langle 110 \rangle$ Si NW with diameter $d = 8$ nm is likewise plotted as a function of the axial strain $\varepsilon_{\parallel}$ in Fig. 5. It also shows a strong dependence on $\varepsilon_{\parallel}$. The highest valence subbands in free-standing $\langle 110 \rangle$ Si NWs have a strong light-hole character. A tensile (resp. compressive) strain tends to reduce (resp. enhance) this light-hole character (Fig. 6), hence the mobility.

Further data, for different diameters and orientations, will be discussed at the conference. The dependence of the electron and hole mobility on the strain is strong whatever the NW orientation. The same trends have been found for the impurity-limited mobility in a Green's functions framework. Strain engineering therefore provides real opportunities to enhance the electrical performances of Si NWs. We will also discuss the accuracy of Boltzmann equation in nanowires.

REFERENCES

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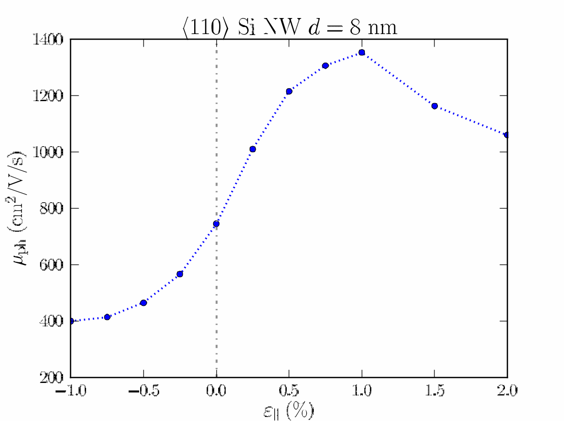

Fig. 1. Electron mobility as a function of axial strain $\varepsilon_\parallel$ in a ⟨110⟩ Si NW with diameter $d = 8$ nm ($T = 300$ K, low carrier concentration).

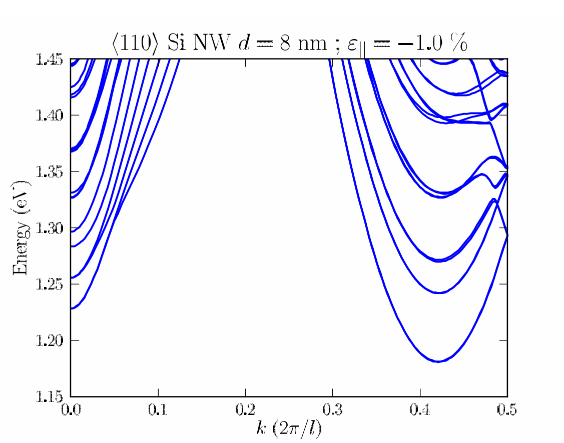

Fig. 2. Conduction band structure of a ⟨110⟩ Si NW with diameter $d = 8$ nm for axial strain $\varepsilon_\parallel = -1\%$.

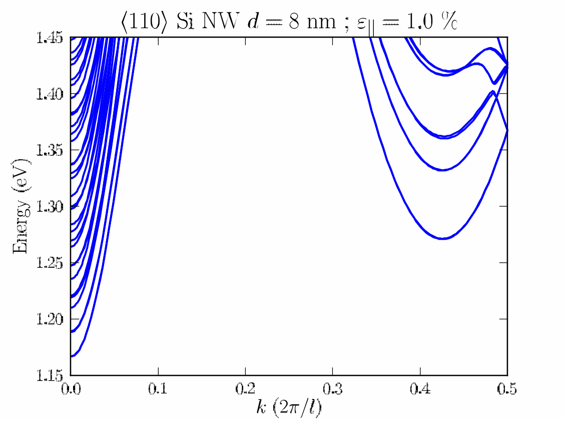

Fig. 3. Conduction band structure of a ⟨110⟩ Si NW with diameter $d = 8$ nm for axial strain $\varepsilon_\parallel = +1\%$.

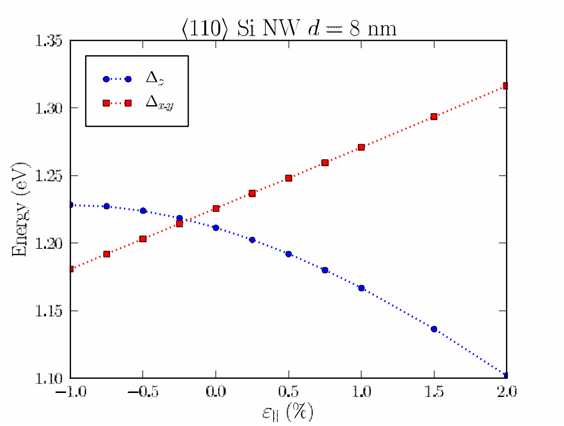

Fig. 4. Energy of the Δ_z and $\Delta_{x,y}$ valleys a function of the axial strain $\varepsilon_\parallel$ in a ⟨110⟩ Si NW with diameter $d = 8$ nm.

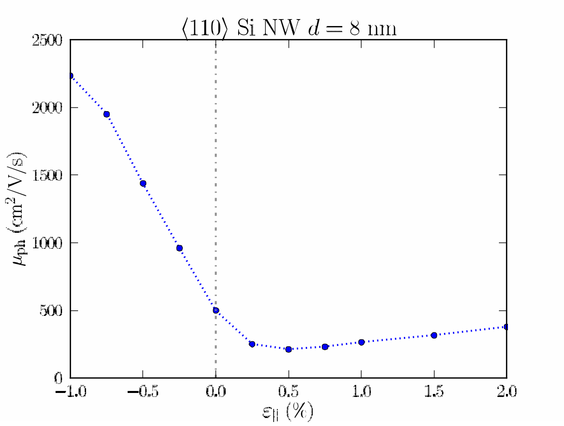

Fig. 5. Hole mobility as a function of axial strain $\varepsilon_\parallel$ in a ⟨110⟩ Si NW with diameter $d = 8$ nm ($T = 300$ K, low carrier concentration).

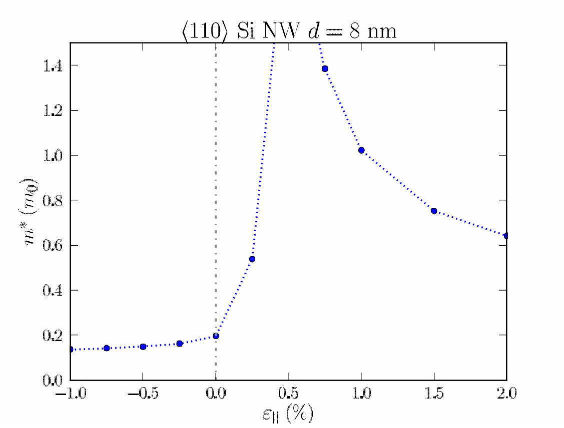

Fig. 6. Hole mass as a function of axial strain $\varepsilon_\parallel$ in a ⟨110⟩ Si NW with diameter $d = 8$ nm.