Shell Strain Effects on Valence Band Structure and Transport Property in Ge/Si$_{1-x}$Ge$_x$ Core-Shell Nanowire

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Introduction

To date, Ge NW based devices are of renewed interest owing to higher bulk mobility with good process compatibility. [1-3]An active area has been improving those NW devices. The realization of core-shell structures with lattice misfit strain offers intriguing chances for improving NW performance. The introduction of strain effects near interfaces can tailor valence band structures. [4] And the optimization of shell materials or compositions during NW heteroepitaxy process is possible to modulate the device property. [5] Si$_{1-x}$Ge$_x$ as a shell based NW device is demonstrated a high performance recently. [6] However, there is a paucity of theoretical study on the strained device performance with a Si$_{1-x}$Ge$_x$ shell in core-shell NWs.

In this work, we calculate the varied strain induced by thickness or Ge contents in shell via finite element method. Then, the strained valence band structure is computed by full 6×6 Luttinger-Kohn Hamiltonian. [6-7] The hole mobility is calculated using modified Kubo-Greenwood formula. [8] The results can help to be a guideline to design NW FETs with core-shell structures.

Simulation Methodology

Based on continuum elastic model, [8] the Si$_{1-x}$Ge$_x$ shell strain energy expression is as follows:

$$U_s = \frac{1}{2} \int d^3x \left( D'_{ij} \left( \epsilon_{ij}^{es} - \epsilon_{ij}^{sc} \right)^2 + \epsilon_{ij}^{es} \epsilon_{ij}^{es} \right)$$

(1)

The core strain energy has a similar form through coordinate transformation. [9] The lattice constant is related to the thickness difference, the shear modulus ratio of Si$_{1-x}$Ge$_x$ shell. [11] And x is the Ge contents in shell. E($\epsilon_{ij}^{es}$) are strain tensor components in Ge core (shell). NWs’ radii in core are fixed 5nm here. The strained valence band structures are calculated via a generalized k·p method and Bessel basis function. [6] Hole density and optical-phonon scatterings are also evaluated. [8]

Results and Discussion

Fig.1 shows strain energy distribution and strain tensor components in Ge (110) NW with 2nm thick Si$_{0.6}$Ge$_{0.4}$ shell. Fig.2 (a) shows valence band structure in pure Ge (110) NW. Compared to NW with 1nm (b) and 2nm (c) thick Si$_{0.6}$Ge$_{0.4}$, strained valence subbands remarkably shift upwards and warps as the shell increases. Fig.3 shows valence band structures in NW with various Ge contents in shell. As the Ge contents reduces from x=0.6 (a) to x=0.4 (b), the valence subbands go up. When the shell is the Si (110) crystal in Fig.3(c), the shifting and warping degree of the subbands is more obvious. Effective masses of top five subbands versus shell thickness and Ge concentration in shell are shown in Fig.4. As the shell becomes thicker, effective masses turn into lower values. But as the Ge contents increases, most effective masses moves larger. Fig.5 plots hole density distribution in Ge NW with 2nm Si$_{0.8}$Ge$_{0.2}$ at 0V, -1V gate voltage. As V$_G$ increases to -1V, the peak hole density in the core increases from $10^{18}$cm$^{-3}$ to $10^{19}$cm$^{-3}$. Fig.6 shows the potential distribution in Ge NW with 2nm Si$_{0.8}$Ge$_{0.2}$ at 0V, -1V gate voltage in a cross section. Fig.7 plots the hole mobility versus effective electric field with 0, 1nm, 2nm thick Si$_{0.8}$Ge$_{0.2}$ shell. The hole mobility is larger with thicker shell. This is caused by larger lattice-misfit strain effects. Fig.8 illustrates the hole mobility versus effective electric field with various Ge contents in shell. The hole mobility increases as the Ge content in shell reduces. NW with Si (110) shell has the largest hole mobility.

Conclusions

Strain induced valence band and hole transport in Ge/ Si$_{1-x}$Ge$_x$ hetero-structure nanowires are investigated. The valence subbands shift upwards and warp as the shell thickness increases or the Ge concentration in shell reduces. The hole mobility with phonon-limited scattering also increases with the thicker shell or lower Ge contents in shell. Our calculation results are useful to optimize the core-shell hetero-structure nanowire performance.

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References

Fig. 1 Strain energy distribution (a) and strain tensor components $\varepsilon_{xx}$ (b), $\varepsilon_{xy}$ (c), $\varepsilon_{yy}$ (d) in Ge (110) NW with 2nm thick Si$_{0.8}$Ge$_{0.2}$ shell (R=5nm)

Fig. 2 Valence band structures in pure Ge (110) NW (a), with Si$_{0.8}$Ge$_{0.2}$ shell: 1nm (b) and 2nm (c)

Fig. 3 Valence band structures in Ge (110) NW with Si$_{0.4}$Ge$_{0.6}$ shell (a), Si$_{0.6}$Ge$_{0.4}$ shell (b) and Si (110) crystal shell (c)

Fig. 4 Effective masses of top 5 subbands in Ge (110) NW versus shell thickness (a), and Ge concentration in shell (b)

Fig. 5 Hole density distribution $\rho(r)$ in Ge (110) NW with 2nm thick Si$_{0.6}$Ge$_{0.4}$ shell at $V_G$=0 (left), $V_G$=-1V (right)

Fig. 6 Cross section of the potential distribution in Ge (110) NW with 2nm thick Si$_{0.6}$Ge$_{0.4}$ shell at $V_G$=0 (left), $V_G$=-1V (right), respectively

Fig. 7 Hole mobility $\mu$ versus effective electric field $E_{eff}$ with different thickness Si$_{0.8}$Ge$_{0.2}$ shell

Fig. 8 Hole mobility $\mu$ versus effective electric field $E_{eff}$ with different Ge contents in 2nm Si$_{1-x}$Ge$_x$ shell