Importance of ionized impurity scattering on resistivity of Si nanowires

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In recent years there have been growing interests in Si and Ge nanowires as promising structures for future electronics.[1] It is advantageous for nanowire FETs since they provide better electrostatic control than planar MOSFETs. However, with regard to carrier transport, nanowire FETs may show drawbacks because, according to the recent experiment by Björk *et al*,[2] resistivity of Si nanowires is found to increase as the nanowire size becomes smaller. For the best performance of nanowire FETs, it is critical to figure out the origin of the increasing resistivity.

The increased resistivity was attributed to the donor deactivation associated with the reduced screening of ionized donors.[2] If this is the case, the reduced screening of the ionized donors may also influence carrier scattering. In this work, scattering effects on the resistivity, with the particular emphasis on the ionized impurity scattering which was neglected in Ref. [2], are investigated through theoretical modeling and numerical simulations.

We consider an infinitely long Si nanowire with cylindrical cross section and radius R_0. In order to explain the experimental results, electrostatic potential is calculated under the condition of the donor deactivation and the charged interface trap between Si and its surrounding oxide with its density D_{it}. In addition, three scattering mechanisms such as acoustic phonon, optical phonon, and ionized impurity scatterings are taken into account. Based on the effective mass equation, a retarded Green's function G^R is obtained self-consistently by solving the Poisson's equation and calculating the self-energies of each scattering. The self-energy of the ionized impurity scattering is given by,

$$\Sigma^{imp}(\vec{r},\vec{r}') = \frac{\omega(\vec{r},\vec{r}')}{2} G^c(\vec{r},\vec{r}') \qquad (1)$$

where $G^c = G^R - G^{R*}$ and $\omega(\vec{r},\vec{r}') = \int d\vec{r}'' n^{imp}(\vec{r}'') v_a(\vec{r}-\vec{r}'') v_a(\vec{r}'-\vec{r}'')$ is the impurity-impurity correlation function with the ionized impurity concentration $n^{imp}(\vec{r})$ and the screened Coulomb potential $v_a(\vec{r})$ in the nanowire environment. For the given Green's function, the resistivity of the system is exactly calculated by evaluating a current-current correlation function.

Typical electrostatic potential and corresponding impurity and carrier distributions are shown in Fig. 1. Due the charged traps, donors at the interface are mostly ionized. The ionized impurity scattering is found to be dominant over the phonon scatterings, which can be seen from the smeared density of states in Fig. 2. The interface trap is also important for determining the electronic resistivity, especially for low carrier concentration (see Fig. 3). This is due to the fact that more ionized impurities induced by the charged interface traps prohibit the propagation of electrons and result in the increased resistivity. With the incorporation of the enhanced impurity scattering as well as the donor deactivation, the results are in good agreement with those of the experiment (see Fig. 4). In order to show their roles on the resistivity, the calculated mobilities and carrier concentration are plotted in Figs. 5 and 6. It is found that the increased resistivity is attributed to both the ionized impurity scattering and the donor deactivation.

REFERENCES

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[2] M. Björk, H. Schmid, J. Knoch, H. Riel, and W. Riess W, *Donor deactivation in silicon nanostructures*, Nature Nanotech. **4**, 103 (2009)

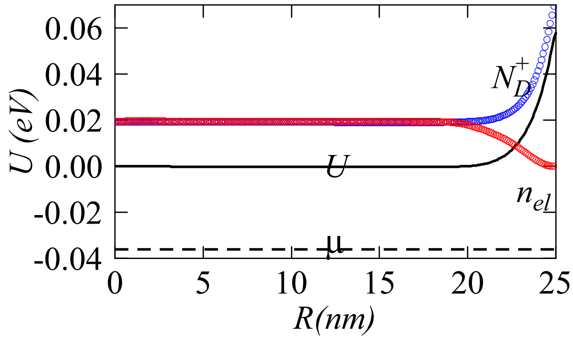

Fig. 1. Calculated potential (solid line), ionized donor N_D^+ (blue circles), and electron n_{el} (red circles) distributions for a nanowire with a radius $R_0 = 25$ nm are plotted for $N_D = 3.0 \times 10^{19}/cm^3$ and $D_{it} = 6.0 \times 10^{12}/cm^2 \cdot eV$.

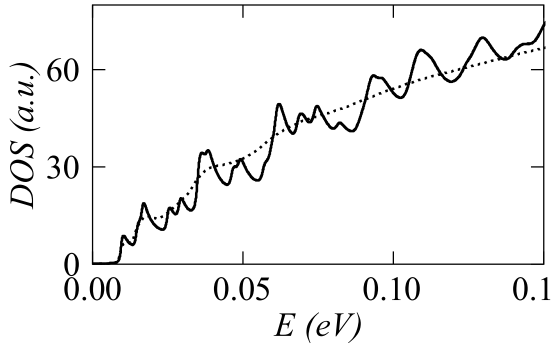

Fig. 2. The densities of state are compared when either phonon (solid) or ionized impurity scatterings (dotted) are present. $R_0 = 10nm$, $N_D = 3.0 \times 10^{19}$, and $D_{it} = 6.0 \times 10^{12}/cm^2 \cdot eV$ are used.

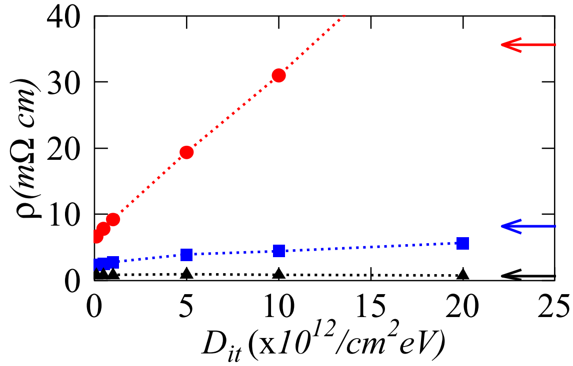

Fig. 3. For a Si nanowire with $R_0 = 15nm$, the variation of the resistivity as a function of D_{it} is shown for the doping concentration $N_D = 9.0 \times 10^{18}$ (red circles), 3.0×10^{19} (blue boxes), and 1.5×10^{20} (black triangles), respectively. Small arrows on the right indicate the expected resistivity from the experiment.[2].

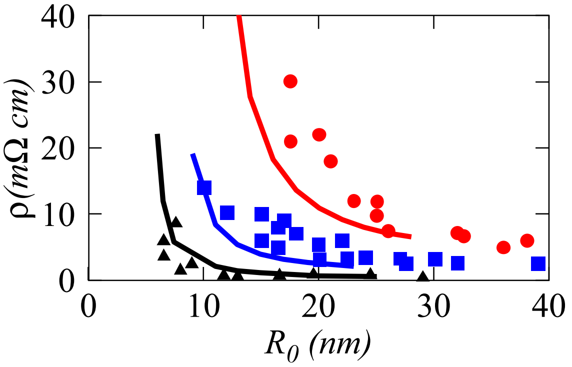

Fig. 4. Calculated resistivity (solid lines) is compared with the experimental result (symbols) of Ref. [2] for doping concentrations $N_D = 9.0 \times 10^{18}$ (red), 3.0×10^{19} (blue), and 1.5×10^{20} (black), respectively. $D_{it} = 6.0 \times 10^{12}/cm^2 \cdot eV$ are used at $T = 300K$.

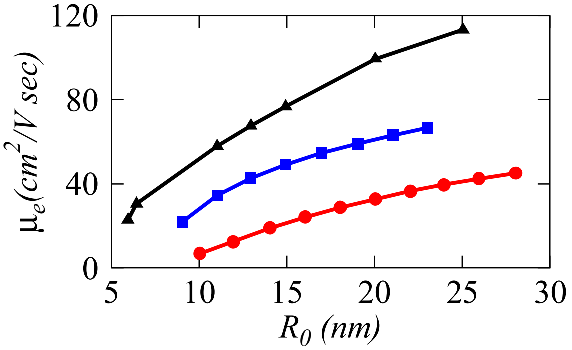

Fig. 5. For $D_{it} = 6.0 \times 10^{12}/cm^2 \cdot eV$ at $T = 300K$, calculated mobilities are plotted as a function of nanowire radius where $N_D = 9.0 \times 10^{18}$ (red circles), 3.0×10^{19} (blue boxes), and 1.5×10^{20} (black triangle).

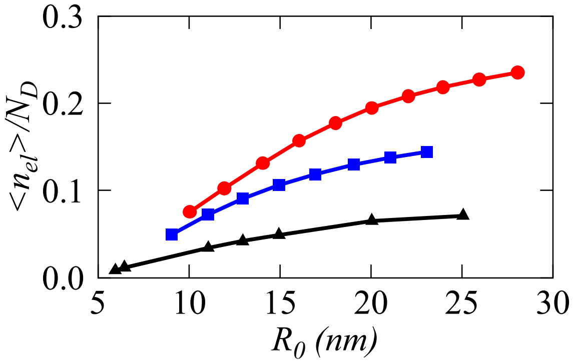

Fig. 6. For $D_{it} = 6.0 \times 10^{12}/cm^2 \cdot eV$ at $T = 300K$, the fractions of carriers to the doping concentration are plotted as a function of nanowire radius where $N_D = 9.0 \times 10^{18}$ (red circles), 3.0×10^{19} (blue boxes), and 1.5×10^{20} (black triangle).