Correlation Effects of Localized Impurities on Electron Transport under 1-D Nano-Structures

N. Sano, M. R. Zulhidza, Y. Kaneno, S. Honda, A. Ueda, and K. Yoshida
Institute of Applied Physics, University of Tsukuba, Tsukuba 305-8573, Japan
E-mail: sano@esys.tsukuba.ac.jp

Abstract. We investigate the spatial correlation effects of ionized impurities on electron transport properties under quasi-1D nanowire structures. The impurity-limited resistance is evaluated with the Landauer formula under various spatial distributions of impurities and the simulation results are theoretically analyzed. We show that phase interference is significant even at room temperature when the separation between impurities along the axis direction is small, whereas strong phase randomization takes place as the separation increases.

1. Introduction
As the device dimension shrinks into nano-scale, the impurity density in the active channel region is inevitably high to attain proper gate-controllability in advanced Si FETs. Nevertheless, the number of impurities in the active region is rather small because of small volume. As a result, transport properties such as mobility could fluctuate, depending on the location and the number of impurities in the channel [1-3]. Such fluctuations in transport characteristics result from both incoherent and coherent effects and quantum mechanical simulations such as the nonequilibrium Green functions (NEGF) method indeed take into account of both effects. However, their physical mechanism is not well explored. In this report, we study numerically and analytically the physics behind the fluctuations of impurity-limited resistances in quasi-1D nanowires.

2. Methodology
2.1. Impurity-limited resistance
According to the Landauer picture, the conductance in quasi-1D nanowires could be calculated from the transmission coefficient through the doped channel region. Since the resistance \( R_{\text{tot}} \) given by the inverse of the conductance thus obtained includes both the quantum (contact) resistance \( R_0 \) and the impurity-limited resistance \( R_s \), \( R_s \) is obtained from \( R_s = R_{\text{tot}} - R_0 \) and expressed by

\[
R_s = \frac{1}{g_{\text{el}}} \frac{\pi \hbar}{e^2} \sum_{l,n} \int_{-\infty}^{\infty} dE \left( 1 - T_{ln}(E) \right) \left( -\frac{\partial f_{\text{F}}(E)}{\partial E} \right) \theta(E - \varepsilon_{ln}) \left\{ \sum_{l,n} \int_{-\infty}^{\infty} dE T_{ln}(E) \left( -\frac{\partial f_{\text{F}}(E)}{\partial E} \right) \theta(E - \varepsilon_{ln}) + \sum_{l,n} \int_{-\infty}^{\infty} dE T_{ln}(E) \left( -\frac{\partial f_{\text{F}}(E)}{\partial E} \right) \theta(E - \varepsilon_{ln}) \right\}.
\] (1)
where $g_{vl}$ is the valley degeneracy, $T_{ln}(E)$ is the transmission coefficient for the in-coming electron in the subband $(l, n)$ with total electron energy $E$ and $\varepsilon_{ln}$ is the subband energy. $f_{FD}(E)$ is the Fermi-Dirac distribution and $\theta(E)$ is the Heaviside step function. Here, we have assumed that there is no “contact” resistance associated with the difference in the local density of states at the junction between the lead and the channel. In other words, we consider the transport properties under the flat potential condition along the axis direction throughout this study. The transmission coefficient $T_{ln}(E)$ is obtained from the Fisher-Lee formula with the retarded Green function calculated by the recursive method. We employ Eq. (1) to calculate $R_s$ in the present numerical simulations.

Under the extreme quantum limit where only the lowest subband $A$ is involved, $R_s$ reduces to

$$R_s = \frac{1}{g_{vl}} \left( 1 - \langle T_A \rangle \right) = \frac{1}{g_{vl}} \frac{\pi \hbar}{e^2} \left( 1 - \langle R_A \rangle \right) \approx \frac{1}{g_{vl}} \frac{\pi \hbar}{e^2} \langle R_A \rangle,$$

(2)

where $\langle T_A \rangle$ and $\langle R_A \rangle$ are, respectively, the transmission and the reflection coefficients weighted with the derivative of the Fermi-Dirac distribution for the in-coming electrons in the lowest subband $A$. The last expression is valid under the weak scattering limit in which $\langle T_A \rangle$ is close to unity. Notice that $R_s$ under the weak scattering limit is bounded above and physically inappropriate. In fact, we can show that the last expression, roughly equivalent to the Born approximation, is identical to the semi-classical expression derived from the Boltzmann transport equation (BTE) under the relaxation time approximation and, thus, the BTE indeed breaks down if the reflection coefficient $\langle R_A \rangle$ is large [4].

2.2. Device structure

For numerical simulations, we employ quasi-1D nanowires with rectangular cross-section area of $3.5 \, \text{nm}^2$ and ionized donor or acceptor impurities are distributed at random in Si channel. The average impurity density in the channel is fixed at $10^{19} \, \text{cm}^{-3}$ so that the channel length $L$ varies according to the number of doped impurities, namely, $L = 8 \, \text{nm}$ for single-impurity, $16 \, \text{nm}$ for two impurities, etc. Since many simulations under various patterns of impurity distributions are required to perform, the scattering potential is assumed to be a simple screened potential (screening length: $\lambda = 1.3 \, \text{nm}$) with image charges associated with the Si/Gate-Oxide interfaces.

3. Results and discussion

3.1. Numerical simulations

We first show numerical simulation results of the impurity-limited resistance $R_s$ for 300 patterns of impurity distributions as a function of the number of (donor or acceptor) impurities in Fig. 1. $R_s$ greatly varies depending on the position of impurities, but the average value of $R_s$’s follows the linear relationship with the channel length and, thus, obeys Ohm’s law. In the case of single-impurity (one impurity is doped in the channel), the fluctuations trivially result from the variations in the subband wave function and the scattering potential of ionized impurity. However, the physics behind such fluctuations for the cases of two and three impurities is rather involved. Figure 2 shows $R_s$ for two donor impurities as a function of the axial separation $\Delta$ between the two impurities. There are three distinct regions, in reference with the averaged resistance indicated by the horizontal dashed line. In region I, fluctuations in $R_s$ are small and most $R_s$’s are close to the average value, which is nearly equal to twice of the resistance for the single-impurity, $2R_{\text{single}}$. As shown in the theoretical analyses below, this is because electron’s phase is rapidly randomized as $\Delta$ becomes longer and the phase among the impurities becomes uncorrelated. Thus, two impurities behave as a series resistance and the total resistance is given by the simple sum of $R_{\text{single}}$ due to each single-impurity. In regions II, $R_s$’s greatly fluctuate and,
in most cases, they are larger than the average value. This implies that the phase interference along the wire axis could play a crucial role even at room temperature. In region III, on the other hand, $R_s$’s become smaller than the average value and this is because the two impurities closely located along the axis direction could be regarded as being on the same transversal plane and, thus, behave as a parallel resistance. It should be noticed that this scenario is possible only if the scattering potential has the long-range part, i.e., the finite screening length.

3.2. Theoretical analyses

In order to clarify the physics involved in $R_s$, let us consider a simple model in which two impurities are doped on the axis of the cylindrical wire and each impurity has the $\delta$-scattering potential in the coordinate space.\footnote{We notice that this simple analytical model is unable to explain the behavior in region III in Fig. 2.}

\begin{equation}
V(R) = v_s(aS)\left\{\delta^{(3)}(R - R_{01}) + \delta^{(3)}(R - R_{02})\right\},
\end{equation}

where $a$ represents the characteristic length along the axis direction over which the scattering potential is effective and $S$ is the cross-sectional area of the wire. $R_{01}$ and $R_{02}$ are the position of impurities. For simplicity, we assume that each impurity has the same scattering potential energy $v_s$. The exact $T_A$ and $R_A$ are calculated from the Lippmann-Schwinger equation and the impurity-limited resistance $R_s$ under the extreme quantum limit is found to be

\begin{equation}
R_s(\Delta) = \frac{1}{g_{sd}} \frac{\pi \hbar}{e^2} \left\{\frac{2\gamma^2(1+\gamma^2)+(1-\gamma^2)\cos(2k\Delta)+2\gamma\sin(2k\Delta)}}{1+2\gamma^2(1+\gamma^2)+(1-\gamma^2)\cos(2k\Delta)+2\gamma\sin(2k\Delta)}}\right\} + \frac{1}{1+2\gamma^2(1+\gamma^2)+(1-\gamma^2)\cos(2k\Delta)+2\gamma\sin(2k\Delta)}),
\end{equation}

where $k$ is the wave number of the in-coming electron and the scattering parameter $\gamma$ is defined by $\gamma = v_s a_{sd}/\hbar k e^2 |\xi_A(0)|^2$ where $\xi_A(r)$ is the subband wave function at radial position $r$.

Figure 3 shows $R_s$ obtained from Eq. (4) as a function of the impurity separation $\Delta$ for $T = 300$ and 30 K. The scattering potential energy is assumed to be $v_s = 183$ meV, corresponding...
to the screening length of $\lambda_{sc} = 2$ nm. The results from the exact expression and the Born approximation are plotted along with $2R_{\text{single}}$ represented by horizontal dashed lines. At low temperature ($T = 30$ K), the oscillatory behavior is clearly seen and this is due to the trigonometric dependence in Eq. (4). This, of course, results from electron’s phase interference between the two impurities. As temperature increases ($T = 300$ K), this oscillation rapidly damps except in the first few nm where $R_s$ is still greatly enhanced by the constructive phase interference. The asymptotic value at large $\Delta$ approaches $2R_{\text{single}}$, which is the uncorrelated limit. Since neither spatial averaging with respect to the position of impurities or energy dissipating scattering such as phonon interaction is included, this phase randomization is caused purely by the broadness in energy spectrum of the in-coming electrons from the reservoir (source). This is confirmed from the temperature dependence of the oscillatory behavior in Fig. 3. As a result, the average of $R_s$ for various $\Delta$ approaches the uncorrelated limit $2R_{\text{single}}$

These findings coincide with those found from the numerical simulations and explain the fact that the constructive interference comes into play in $R_s$ even at room temperature if the impurity separation is small and that $R_s$ rapidly approaches the average value as the separation becomes larger. In addition, we should point out that the Born approximation completely breaks down at room temperature.

4. Conclusions
We have investigated numerically and theoretically the spatial correlation effects of ionized impurities on electron transport under the nanowire structures. We have demonstrated explicitly how the phase interference and phase randomization take place simultaneously in the impurity-limited resistance $R_s$ at room temperature. Namely, the constructive phase interference is dominant even at room temperature in $R_s$ if two impurities are located close each other, whereas $R_s$ rapidly approaches the uncorrelated limit as the separation becomes larger. As a result, the ensemble average resistance follows classical Ohm’s law even under nanostructures.

References
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