Impact of Discrete Dopant in Source and Drain Extensions on Characteristics of Nanowire Transistors: KMC and NEGF Study

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Intrinsic parameter fluctuation due to random impurities is becoming a major concern for continuously scaled down metal-oxide-semiconductor field-effect-transistors (MOSFETs) [1]. For ultra-small MOSFETs, not only random location of individual dopant atoms but also fluctuation of number of active impurities is expected to have significant impacts on the device performance. Here we have studied effects of discrete dopant in source and drain (S/D) extensions on characteristics of silicon nanowire (Si NW) transistors by using kinetic Monte Carlo (KMC) simulators for generating distribution of active dopant atoms and by using non-equilibrium Green's function (NEGF) method for calculating current-voltage characteristics.

Discrete impurity distribution in a Si NW was calculated using KMC simulators based on DADOS (Diffusion of Atomistic Defects, Object Oriented Simulator) [2]. Figure 1 shows discrete boron (B) distribution in a Si NW (10 nm width, 30 nm length) with 1 nm-thick oxide calculated by UVAS (University of Valladolid Atomistic Simulator) [3]. The Si NW was implanted with B (1 keV, $1 \times 10^{15}\,\mathrm{cm}^{-3}$) and annealed at 1,000 °C for 10 s. Most of the B atoms are in the oxide, at the oxide/Si interface, and in B clusters, and only about 10 % B atoms are found to be active in Si. The B activation ratio decreases with smaller width of NW. In addition, arsenic (As) distribution in a Si NW (3 nm width, 10 nm length) with 1 nm-thick oxide was calculated using the Sentaurus KMC simulator [4]. The Si NW was implanted with As (0.5 keV, $1 \times 10^{15}\,\mathrm{cm}^{-3}$) and annealed at 1,000 °C with hold time of 0 s. Statistical variations are investigated by using 200 different random seeds. In a similar manner to B, most of the As atoms are in the oxide, at the interface, and in As clusters, and only ~30 As atoms are active in a Si NW (see Fig. 2).

The active As distributions obtained through KMC simulation are introduced into S/D extensions of n-type Si NW MOSFETs, whose device structure is given in Fig. 3. The drain-current–gate-voltage (I_d–V_g) characteristics were calculated by NEGF method with an effective mass approximation [5]. The discrete impurities are treated with a cloud-in-cell charge assignment scheme. Figure 4 shows I_d–V_g characteristics of 100 devices with different discrete impurity distributions, together with a continuously doping case in S/D extensions for comparison (see also Fig. 5 for carrier density profiles and location of active As atoms in some representative devices). The drain current was found to be reduced compared to that with uniform As distribution. The normalized average current $\langle I_\mathrm{d}\rangle/I_0$ (I_0 is the drain current of the continuously-doped device) is found to be ~0.8 and decreases with V_g (see Fig. 6). We also find that the standard deviation of the 100 samples is $\sigma I_\mathrm{d} \approx 0.2\langle I_\mathrm{d}\rangle$.

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[1] S. Roy and A. Asenov, Science **309**, 388 (2005).
[2] I. Martin-Bragado, "Process atomistic simulation for microelectronics," Doctoral thesis, University of Valladolid (2004).
[3] UVAS Help, University of Valladolid (2006).
[4] Sentaurus Process User Guide, Version F-2011.09, Synopsys, Inc. (2011).
[5] H. Takeda and N. Mori, J. Comput. Electron. **4**, 31 (2005).

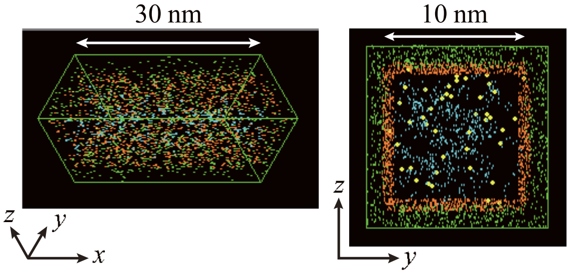

Fig. 1. Discrete boron (B) distribution in a Si NW (10 nm width, 30 nm length) calculated by UVAS; (left) entire and (right) cross sectional view. The Si NW was implanted with B (1 keV, 1×10^{15} cm^{-3}) and annealed at 1,000 °C for 10 s. Yellow dots show active B atoms in Si.

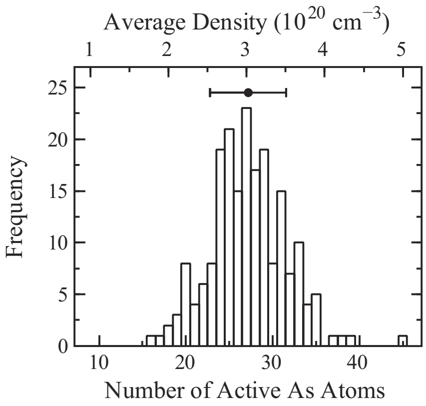

Fig. 2. Histogram of number of active arsenic (As) atoms in a Si NW (3 nm width, 10 nm length) calculated by the Sentaurus KMC simulator. The Si NW was implanted with As (0.5 keV, 1×10^{15} cm^{-3}) and annealed at 1,000 °C with hold time of 0 s. 200 different Si NWs are simulated.

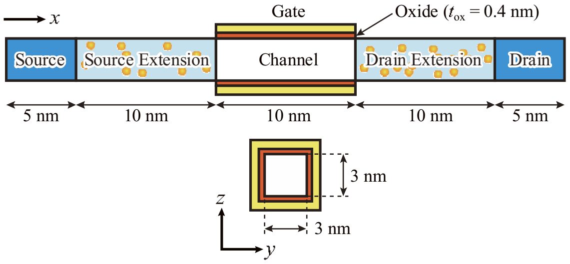

Fig. 3. Schematic diagram of the n-type Si NW MOSFET. Discrete distributions of the active As atoms are introduced into the S/D extensions. To mimic metal electrodes, the S/D regions are heavily doped with $N_d = 5{\times}10^{20}$ cm^{-3} (continuously doping). The channel region is intrinsic. We simulated 100 samples using 200 different random seeds (each sample needs 2 random seeds for S/D extensions).

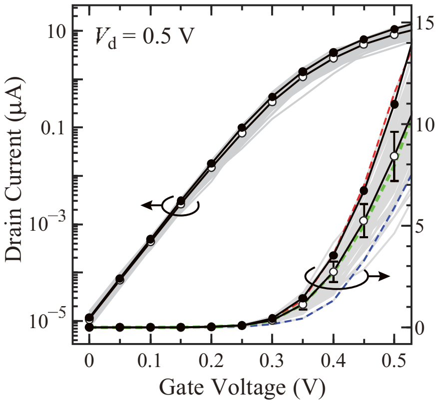

Fig. 4. I_d–V_g characteristics at V_d = 0.5 V. Gray lines show I_d–V_g of 100 samples with different discrete impurity distributions. Open circles represent their average value $\langle I_d \rangle$. Continuously doping case with $N_d = 3{\times}10^{20}$ cm^{-3} in S/D extensions is shown by solid circles for comparison.

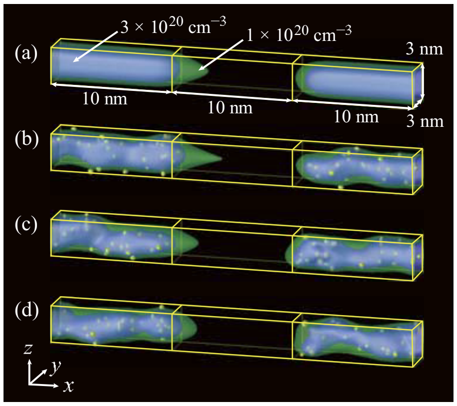

Fig. 5. Equidensity surfaces (blue and green surfaces) and impurity positions (yellow dots) for (a) continuously-doped, (b) high-current [red dashed line in Fig. 4], (c) medium-current [green], and (d) low-current [blue] devices. $V_d = V_g$ = 0.5 V.

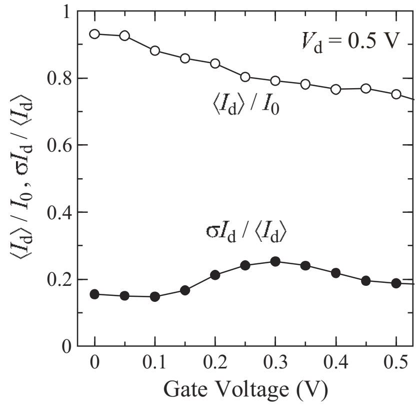

Fig. 6. Average current $\langle I_d \rangle$ and standard deviation σI_d *vs* V_g. I_0 is the drain current of the continuously-doped device.