1. Introduction

As the scaling of Si-MOSFETs has brought the device size into the deep sub-μm regime, fluctuations of various device properties have become one of the critical issues for future device technology [1-2].

In particular, threshold voltage variation due to fluctuations of the number and location of dopants has received great attention recently [3-7]. In most cases, the dopant variation is studied within the framework of the conventional jellium dopant model, in which the variation of the dopant concentration at each mesh changes smoothly [3-6]. It should be emphasized, however, that the discreteness of dopants cannot be overlooked in sub-0.1 μm Si-MOSFETs, because each mesh employed in 3-D simulations contains no dopant or, at most, one dopant in the channel regions. It is, therefore, no longer possible to regard the dopants as jellium, but rather their localized characteristics in 3-D space have to be explicitly taken into account.

In the present paper, we investigate the statistical threshold fluctuations in sub-0.1 μm Si-MOSFETs via fully 3-D Drift-Diffusion (DD) simulations with emphasis on the atomistic nature of both donors and acceptors. It is demonstrated that the subthreshold characteristics are strongly dependent of the dopant model (either jellium or atomistic) and shifted to the higher gate voltages in the case of the atomistic dopants, which is a sharp contrast to the results reported before.

2. Atomistic Dopant Simulation Model

The 3-D DD simulations are carried out under a typical n-channel Si-MOSFET structure. The device parameters employed in the simulations are summarized in Table 1. Since the electric potential resulting from a localized dopant is polar symmetric, it is mandatory to use an isotropic mesh. In the present study, a cubic mesh with the length Δx = 2 nm is employed in the entire device regions. The discretized dopants are then generated inside each cubic mesh, in accordance with the Poisson distribution [3]. Figure 1 shows a typical dopant (both donor and acceptor) distribution generated in the n-channel Si-MOSFET used for the following simulations. The numbers of donors and acceptors inside the device are 4237 and 763, respectively. The dopant concentration at each mesh node is calculated from the number of dopants inside the mesh, which is, at most, one in many meshes. Note that this is equivalent to replacing the dopant concentration in the right-hand-side of the Poisson equation by the atomistic δ-function.

3. Simulation Results and Discussion

Figure 2 shows the subthreshold characteristics obtained from the DD simulations under the four different dopant models: conventional uniform 2-D model, 2-D

| channel length $L_{efl}$ (nm) | 50 |
| device width $W$ (nm) | 50 |
| oxide thickness $t_{ox}$ (nm) | 3 |
| (uniform) substrate impurity $(\text{cm}^{-3})$ | $1 \times 10^{18}$ |
| junction depth $x_j$ (nm) | 10 |

Table 1: Device parameters employed for the 3-D Drift Diffusion simulations.
jellium model, fully (both donors and acceptors) atomistic model, and atomistic acceptor model. Notice that the dopant distribution shown in Fig. 1 is fixed and the dopant concentration at each mesh node is varied according to the dopant model. It is clear that the subthreshold characteristics are strongly dependent of the dopant model employed and shifted to the higher gate voltages in the case of the atomistic dopants.

The shift of the subthreshold characteristics may be explained as follows. The electronic potential due to a localized acceptor becomes a sharp peak in the channel and the channel electrons ought to keep away from such a peak to flow from the source to the drain. In other words, the regions of electrons flowing in the channel are restricted and the channel becomes more resistive. As a result, larger gate voltages are required to suppress the potential barrier in the channel. Figure 3 shows the electronic potential configurations underneath the gate oxide in the n-MOSFET. There are three localized acceptors in this plane, which greatly restrain an electron from flowing in the channel.

Very recently, Asenov has investigated the threshold variations from the viewpoint of atomistic acceptors [7]. He has employed a simplified 3-D simulation scheme, in which the electronic current-continuity equation is decoupled with the 3-D Poisson equation. His results also show that the potential configuration inside the device is greatly inhomogeneous. Nevertheless, the averaged threshold voltage becomes slightly smaller (≈ 50 mV) than that of conventional 2-D DD simulations. We believe that this contradiction comes from whether the self-consistent treatment of the current-continuity equations is made. In fact, it is always necessary to include the self-consistency to achieve good convergence in our simulations. However, we do not claim that the present results are quantitatively correct, because of an inaccurate treat-

4. Conclusions

The statistical threshold fluctuations in sub-0.1 μm Si-MOSFETs have been investigated via the 3-D Drift-Diffusion simulations with emphasis on the atomistic nature of both donors and acceptors. It has been found that the subthreshold characteristics are strongly dependent of the dopant model employed and shifted to the higher gate voltages in the case of the atomistic dopants.

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