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Ensemble Monte Carlo/Molecular Dynamics Simulation of Inversion Layer Mobility in Si MOSFETs — Effects of Substrate Impurity

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Abstract — **Electron transport in bulk Si and MOSFET inversion layers is studied using an ensemble Monte Carlo (EMC) technique coupled with the molecular dynamics (MD) method. The Coulomb interactions among point charges (electrons and negative ions) are directly taken into account in the simulation. It is demonstrated that the static screening of Coulomb interactions is correctly simulated by the EMC/MD method. Furthermore, we calculate the inversion layer mobility in Si MOSFETs, and mobility roll-off near the threshold voltage is observed by the present approach.**

I. INTRODUCTION

The low-field carrier mobility is a key that determines the performance of scaled Si-MOSFETs [1]. Coulomb scattering is one of the most important limiting factor for carrier transport, but evaluation of its effect in small devices is very complex; e.g., not only the local channel dopants but also the remote ions in the source [1] and the gate [2, 3] cause the reduction of the channel mobility in sub-100 nm MOSFETs. Therefore, the accurate numerical simulation of Coulomb interactions taking account of screening effect is essential to predict the performance of future MOSFETs.

The ensemble Monte Carlo (EMC) simulation coupled with the molecular dynamics (MD) method has been previously reported as a technique to treat complicated Coulomb interactions among electrons and ionized impurities in semiconductors [4, 5, 6]. In the present study, we verify the validity of EMC/MD method through the simulations of electron transport in the simple test structures. Firstly, we analyze the low-field electron transport in bulk-Si in which negative ions are doped. We then apply the EMC/MD approach to the calculation of inversion layer mobility in n-MOSFETs limited by substrate acceptor ions [7].

II. SIMULATION IN BULK SILICON

Figure 1 shows the simulation system considered. In this study, our interest is concentrated in the analysis of the minority carrier transport in p-Si, and hence the particles put into the system are the mobile electrons and the fixed ionized acceptors. Because both particles are negatively charged, we can avoid the serious problem

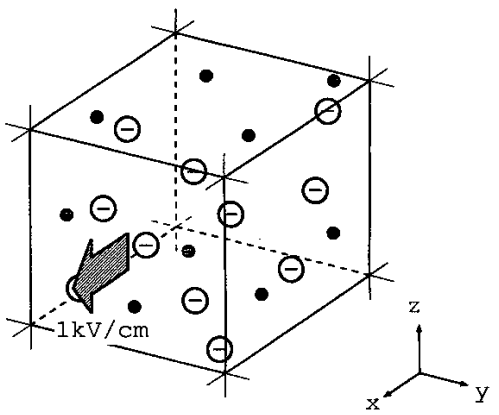

Figure 1: Schematic view of the simulation system for electron transport in bulk-Si. Ionized acceptors (open circles) and electrons (dots) are randomly placed inside a box, and 3D periodic boundary condition is imposed. An external field of 1 kV/cm is applied to x-direction.

pointed out to the EMC/MD method, i.e., the electron trapping by the positive ions [5]. The Coulomb force acting on the electron i, $\mathbf{F}_i$, is calculated by summing all the forces exerted by other point charges j:

$$\mathbf{F}_i = \sum_j \frac{e^2}{4\pi\epsilon_{\rm Si}|\mathbf{r}_i - \mathbf{r}_j|^2}\,, \qquad (1)$$

where e is the elementary charge, $\epsilon_{\rm Si}$ is the permittivity of Si, and $\mathbf{r}_i$ is the position of the ith particle. The standard EMC model [8] is employed for all other physics regarding the electron transport, i.e. the electron-phonon scattering, the anisotropic effective mass, the non-parabolicity of band structure, etc. The maximum number of simulated electrons is 2,000. Their trajectories influenced by the internal and external fields are tracked with a time step of 0.1 fs.

Figure 2 shows the calculated electron mobility at room temperature. The mobility drops with decreasing the electron concentration, indicating that the screening effect works well in the EMC/MD simulation.

Figure 3a plots the potential energy distribution from the ions in the simulated system. When electrons are brought into the system, the potential fluctuation is of course enhanced as shown in Fig. 3b. However, the electron-electron (e-e) interactions do not directly affect the mobility, because the total momentum is conserved before

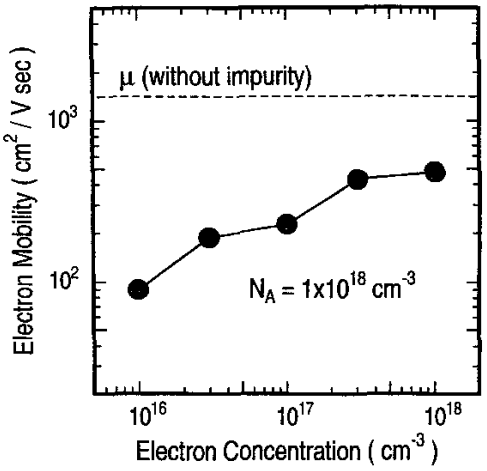

Figure 2: Calculated mobility of electrons in bulk-Si as a function of electron concentration. The ionized impurity (acceptor) concentration is 10^{18} cm^{-3}, and the lattice temperature is 300 K.

and after the e-e collision. Figure 3c plots the potential distribution averaged over 2 ps. Note that the long wave length component of the potential fluctuation shown in Fig. 3a is weakened, or screened, by the electrons which are distributed away from the ions. The uneven electron distribution is clearly observed in the time-averaged simulation results as shown in Fig. 4.

In Fig. 5, the power spectral density (PSD) of the potential energy fluctuation is analyzed using FFT. We compared the PSD of the potential energy from ionized impurities only (see, Fig. 3a), $S_{\rm ion}(q)$, and the PSD of the time-averaged potential taking account of mobile electrons as well as fixed impurities (see, Fig. 3c), $S_{\rm ion+e}(q)$. Due to the Coulombic nature of the ion's potential energy, $S_{\rm ion}(q)$ decreases with q as $S_{\rm ion}(q) \propto q^{-4}$. However, the long wave length component of $S_{\rm ion+e}(q)$ is damped by the screening effect. A significant damping appeared at q smaller than the Debye-Hückel's screening parameter [9]:

$$q_s = \sqrt{\frac{e^2 n}{\epsilon_{\rm Si} k_B T}} , \qquad (2)$$

where n is the electron concentration. In Fig. 6, the ratio between the PSDs of the bare and screened potentials is shown; we plot $[S_{\rm ion}(q)/S_{\rm ion+e}(q)]^{1/2}$ as a function of q. The simulated result is consistent with the analytically derived expression for the low-frequency dielectric function [9]:

$$\epsilon(q, \omega \to 0) = 1 + \frac{q_s^2}{q^2} . \qquad (3)$$

As is discussed above, the static screening of the Coulomb interactions by the mobile electrons is correctly simulated by the EMC/MD method.

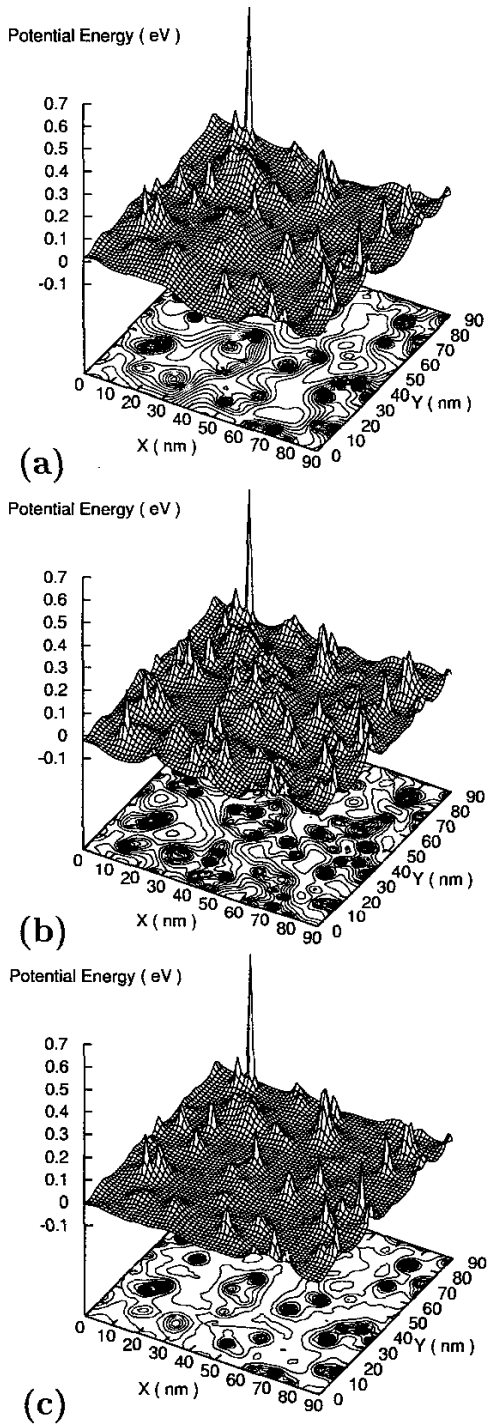

Figure 3: Potential energy distribution in xy plane. (a) From ionized impurities only ($N_{\rm A} = 10^{18}$ cm^{-3}). (b) Snap shot during the simulation with $N_{\rm A} = 10^{18}$ cm^{-3} and $n = 10^{18}$ cm^{-3}. (c) Time-averaged potential distribution during the simulation for 2 ps.

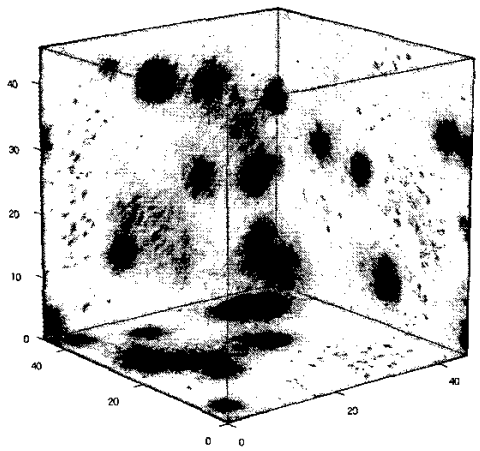

Figure 4: Time-averaged distribution of simulated electron concentration inside a box, 46 nm each side. The dark area corresponds to the low electron concentration region, near where the negatively charged ions exist. The concentrations of impurities and electrons are both 10^{18} cm^{-3}.

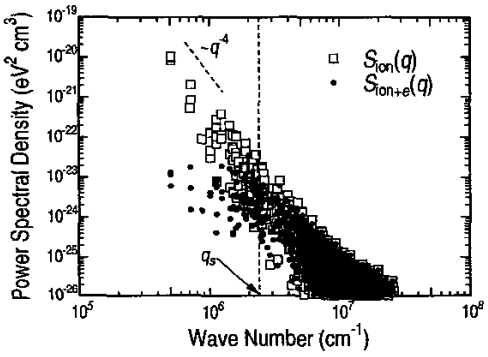

Figure 5: Power spectral density of the potential energy fluctuation inside a simulation region; potential energy from ionized impurities only (open squares), and time-averaged potential taking account of mobile electrons as well as fixed impurities (dots). The concentrations of impurities and electrons are both 10^{18} cm^{-3}. The lattice temperature is 300 K. The screening parameter q_s estimated by Debye-Hückel model is indicated by an arrow, and the dependence proportional to q^{-4} is shown by a dashed line.

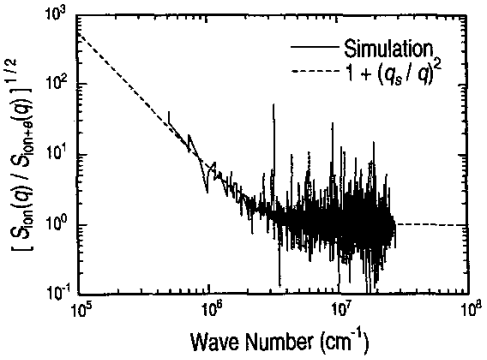

Figure 6: $[S_{\rm ion}(q)/S_{\rm ion+e}(q)]^{1/2}$ is plotted as a function of q. The dashed line shows the analytic expression for the low-frequency dielectric function.

III. SIMULATION OF ELECTRON TRANSPORT IN INVERSION LAYERS OF N-MOSFET

We applied the EMC/MD method to the simulation of electron transport in Si-inversion layers. Figure 7 shows schematic of the unit cell for the simulated system. The external field along z-direction is applied, and 2D periodic boundary condition is imposed to x- and y-directions. The Coulomb force acting on the ith electron located at $\mathbf{r}_i$ is calculated by summing all the forces exerted by other point charges at $\mathbf{r}$ within a cut off range:

$$|r_x - r_{x,i}| < L/2, \quad |r_y - r_{y,i}| < L/2 \,, \tag{4}$$

where L is the size of the unit cell. Due to the long-range nature of Coulomb interaction, this cut-off procedure causes the non-negligible effects on the simulation results. In the present study, we treated the charges outside the cut off region as continuous, and the electric field from the continuous charge are calculated by analytical integration, which modifies the vertical force acting on the electron [6]. In order to include a polarization effect at the Si/SiO_2 interface, we take account of the Coulomb interactions with not only the *real* charges but also the image charges induced in SiO_2 layer [6]. The number of particles introduced into the system is determined by the following way. Firstly, we give the substrate doping density N_A and the oxide field $E_{\rm ox}$. We calculate the depletion layer width x_d as

$$x_d = \sqrt{\frac{2\epsilon_s \Psi_s}{eN_A}} \,, \tag{5}$$

where Ψ_s is the band bending in the substrate depletion layer. Ψ_s is approximated as

$$\Psi_s = 2\Psi_B \tag{6}$$

$$= 2\frac{k_B T}{e} \ln\left(\frac{N_A}{n_i}\right) \tag{7}$$

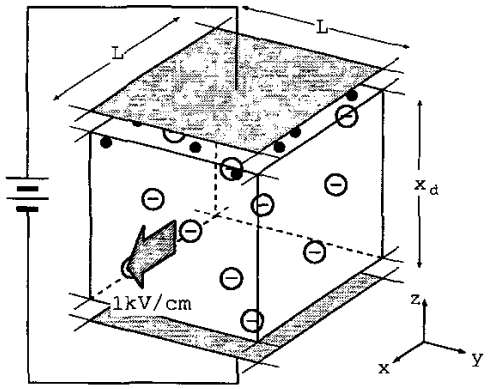

Figure 7: Schematic view of the simulation system for electrons in MOSFET inversion layer. 2D periodic boundary condition is imposed. External fields are applied to x- and z-directions.

where Ψ_B is the potential difference between the Fermi level and the intrinsic Fermi level, and n_i is the intrinsic carrier density. Number of ionized impurities in the substrate is then given by $x_d N_A L^2$, and the number of electrons is $(\epsilon_{ox} E_{ox}/e - x_d N_A) L^2$.

Figure 8 shows the calculated mobility as a function of effective normal field, $E_{\rm eff}$, defined as:

$$E_{\rm eff} = \frac{e}{\epsilon_{\rm Si}} \left(N_d + \frac{1}{2} n_s \right) , \qquad (8)$$

where N_d is the surface concentration of the depletion charge, n_s is the surface inversion carrier concentration. The mobility drop is observed near the threshold of the inversion layer formation [7]. If the higher gate voltage is applied, electrons are pushed up to the interface, and the surface electron concentration increases. Thus, the screening effect works to raise the electron mobility.

IV. CONCLUSION

In summary, we have simulated the low-field electron transport in bulk-Si and Si inversion layers by using the EMC/MD method, and verified its validity to treat the Coulomb interactions in the devices. It has been demonstrated that the screening effect and the mobility roll-off of the inversion electrons are well simulated by the present approach. The EMC/MD is a useful approach to simulate the complex Coulomb interactions in the small semiconductor devices.

ACKNOWLEDGEMENT

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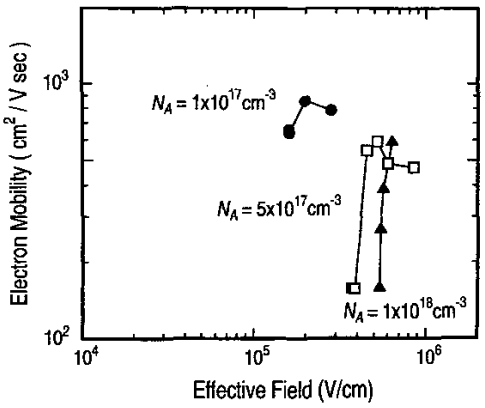

Figure 8: Calculated inversion layer mobility vs. effective field characteristics at 300 K as a parameter of substrate carrier concentration, N_A.

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