Ensemble Monte Carlo/Molecular Dynamics Simulation of Electron Mobility in Silicon with Ordered Dopant Arrays

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Abstract—**Electron transport in bulk silicon with ordered dopant arrays is studied using an ensemble Monte Carlo (EMC) technique coupled with molecular dynamics (MD) method. This work is motivated by a recently developed single-ion implantation (SII) technique, which enables us to fabricate a semiconductor device with an ordered dopant array. We numerically estimate the carrier mobility in silicon with such an ordered dopant array comparing to that with conventional random dopant distribution. The calculation results show that electron mobility can be enhanced in the ordered dopant array if the fluctuation of dopant position is less than 5 nm.**

Keywords - Single Ion Implantation; Ordered Dopant Arrays; Electron Mobility; Coulomb Scattering

I. INTRODUCTION

Random distribution of dopant atoms produced by the present ion implantation technique inevitably causes fluctuation in devise parameters, which is becoming a major issue in scaling and integration. Recently, a novel ion implantation method, named Single Ion Implantation (SII) [1], was developed by a part of the authors to precisely control the number and position of the dopant atoms. In the SII method, single ion is extracted by chopping a focused ion beam using a small aperture and high frequency beam deflection and then injected into the aimed point in a substrate. This technique enables us to fabricate a semiconductor device with well ordered dopant arrays. It has been demonstrated that the device-to-device fluctuations in the conductance and threshold voltage are actually suppressed by the ordered dopant arrays compared to the conventional random dopant distribution [2, 3].

Such an ordered dopant array alters also intrinsic characteristics of the semiconductor devices. It was found that the devices with the ordered dopant arrays exhibit a larger shift in threshold voltage than that for a random dopant distribution [3]. This is attributed to the difference in the uniformity of electrostatic potential in the conducting channel region between the ordered and random distributions of dopant atoms.

It is further expected that the carrier mobility in the device with ordered dopant array is enhanced because the impurity scattering would be reduced in such a uniform electrostatic potential, although it has not yet been demonstrated with the aiming accuracy of the present SII technique [4]. To estimate how much accuracy is required to observe an enhancement of the carrier mobility, it is essential to use an advanced carrier transport simulation which takes into account the discreteness of charge and atomicity of dopant distribution.

So far, the discreteness of dopant atoms have been considered in the drift-diffusion (DD) simulation [5] and ensemble Monte Carlo (EMC) technique coupled with molecular dynamics (MD) [6]. The effect of the periodic dopant array also has been studied by quantum mechanical analysis [7] and it has been predicted that the scattering probability of electron would be reduced due to the electron wave interference. However, there are no reports on the carrier transport analysis supposing a practical ordered dopant array where each dopant atom is displaced from an exact periodic position.

In this work, we perform a series of EMC/MD simulation in order to numerically estimate the carrier mobility in silicon with an ordered dopant array taking the fluctuation of dopant position into account.

II. SIMULATION METHOD AND MODEL

In the EMC/MD method, the carriers are treated as classical particles, and their real-space trajectories are simulated by the classical MD method, which solves the Newtonian equation of motion under the bare Coulomb potential among point charges of carriers and dopant ions. Phonon scattering is simulated as stochastic changes in the momentum of carriers by the EMC algorithm [8, 9].

In the present simulation, the particles put in the system are the mobile electrons and the fixed ionized acceptors, and both particles are negatively charged modeling an inversion layer of p-type Si. The acceptor ions are arranged in a cubic lattice of 10 x 10 x 10 lattice points with an interval of d, and a small fluctuation is imposed to the dopant arrangement to reflect the

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aiming precision of SII in the simulation. The fluctuation of the dopant arrangement is assigned randomly according to a Gaussian distribution centered at each lattice point with a specified standard deviation σ. All electrons are randomly distributed within the simulation box called a unit cell, on which a three-dimensional periodic boundary condition was imposed. It is supposed that the unit cell is surrounded by its replicas. The simulation system considered is illustrated in Figure 1. The concentration of electron and ion are determined by the number of each particle. An external field of 1 kV/cm is applied to the *x*-direction.

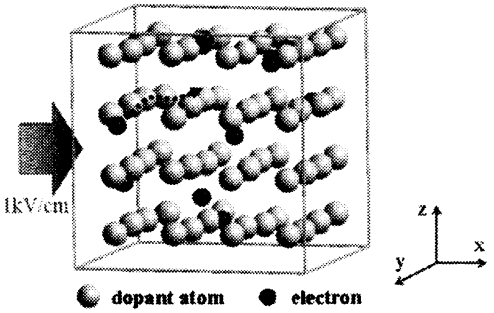

Fig.1 Schematic view of the simulation system for electron transport in Si with ordered dopant array.

In the MD procedure, the forces acting on an electron comprise the interparticle force and the external force of the applied field. The interparticle force is computed by summing all the repulsive Coulomb force exerted by other particles inside the unit cell and the adjacent replicas within the cut-off range. In this study, the cut-off range is defined as

$$|x-x_i|<\frac{L}{2},|y-y_i|<\frac{L}{2},|z-z_i|<\frac{L}{2}, \quad (1)$$

where L is the side length of the unit cell. The long range component is supposed to be zero in this work, because we approximate the charge outside cut-off range as continuous and uniformly distributed [6]. To integrate the Newtonian equation of motion, we use the leapfrog scheme and the time step used is 0.1fs. Thus the time evolution of electron ensemble is simulated, and the electron mobility is evaluated by averaging the electron velocities over time. The simulation is performed for a long time enough to reach the convergence.

Even though the long range Coulomb force is omitted, the most time-consuming task in the MD simulation is still the calculation of the Coulomb interaction between each pair of charged particles. The amount of the calculation increases in proportion to the square of the number of charged particles. To accelerate the calculation of the Coulomb forces, we utilize MDGRAPE-3 [10] which is a petaflops special-purpose computer for MD simulations.

The standard EMC model [8, 9] is employed to describe all other physics regarding the electron transport. Six equivalent *X*-valleys of conduction band are expressed by ellipsoidal non-parabolic band model, which is represented as

$$E(1+\alpha E)=\frac{\hbar^2}{2}\left[\frac{(k_x-k_{x0})^2}{m_x}+\frac{(k_y-k_{y0})^2}{m_y}+\frac{(k_z-k_{z0})^2}{m_z}\right], \quad (2)$$

where m_x, m_y, and m_z are each axial effective mass. Two of such effective masses are transverse effective masses: $m_t = 0.19\ m_0$. One of them is longitudinal effective mass: $m_l = 0.98\ m_0$. k_{x0}, k_{y0}, and k_{z0} are center of *X*-valley coordinate (wave number vector in case that energy takes minimum value). α (=0.5 eV^{-1}) is a nonparabolicity parameter.

III. Results and Discussion

Figure 2 shows the calculated electron mobility with the EMC/MD simulation as a function of the standard deviation σ of the fluctuation in the dopant array. The concentration of the acceptor ions (N_A) is set to 10^{18} cm^{-3} (d = 10 nm), and we calculate three cases with different electron concentrations (n) of 10^{17} cm^{-3}, 10^{18} cm^{-3}, and 10^{19} cm^{-3}. It is revealed that if σ < 5 nm, the electron mobility is enhanced when the electron concentration is equal to or smaller than that of the acceptor ions. As σ increases, the mobility converges to the value in the randomly distributed dopants.

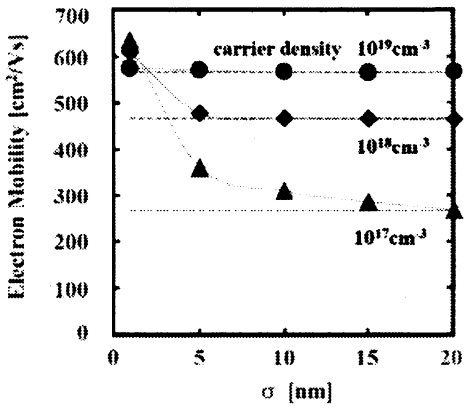

Fig.2 Calculated mobility of electrons as a function of σ of the dopant array. The concentration of the acceptor ions is set to $10^{18}cm^{-3}$. Dashed lines show the motilities in the randomly distributed dopants.

Figure 3 shows the density profile of the projected trajectories of whole electrons onto the *y*-*z* plane which is perpendicular to the direction of the electric field. The dark area corresponds to the high electron concentration region. Figure 3a shows the electron distribution in a randomly distributed acceptor ions, where electrons are locally concentrated. Contrarily, in a well ordered dopant arrangement with σ = 1 nm, as shown in Fig. 3b, the electrons are uniformly distributed over the system except for the proximity of the acceptor ions.

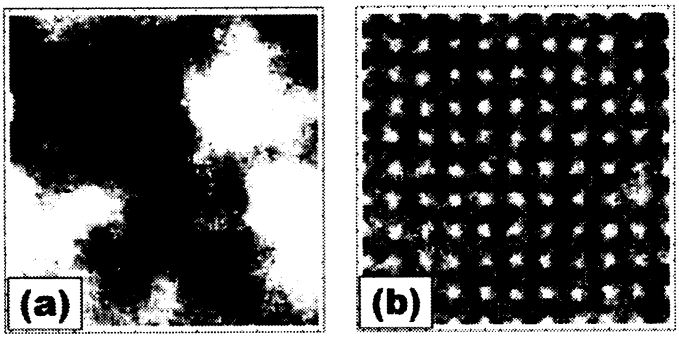

Fig.3 Distribution of simulated electron in (a) a randomly distributed dopant ions, and (b) in an ordered dopant arrangement with σ = 1 nm. Dark area corresponds to the high electron concentration region.

Figure 4 summarizes the estimated electron mobility for various acceptor ion concentrations: N_A = 10^{15} cm^{-3}, 10^{16} cm^{-3}, 10^{17} cm^{-3}, and 10^{18} cm^{-3}. For each concentration of acceptor ions, we test three cases with different electron concentrations; the assumed electron concentrations are equal to, 10 times as much as, and one-tenth of the acceptor ions. The results show that the electron mobility does not depend on σ for the lower dopant concentrations of 10^{15} cm^{-3} and 10^{16} cm^{-3}. At the higher dopant concentrations of 10^{17} cm^{-3} and 10^{18} cm^{-3}, if the electron concentration is greater than that of the dopant atoms, the electron mobility is almost constant irrespective of the value of σ. Thus the electron mobility enhancement by the ordered dopant placement becomes obvious when the dopant concentration is larger than about 10^{17} cm^{-3} and the electron concentration is lower or equal to that of the dopant atoms.

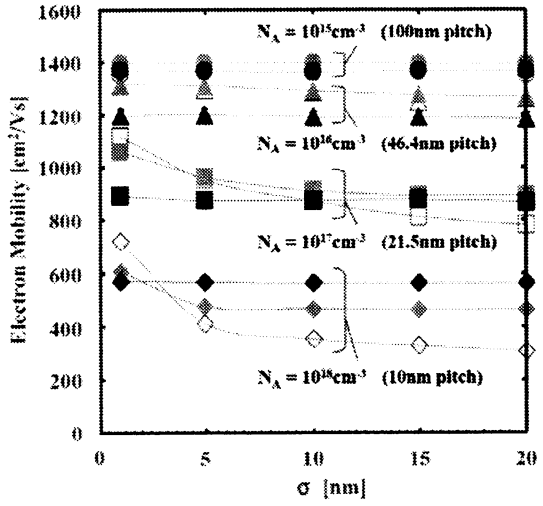

Fig.4 Calculated mobility of electrons as a function of standard deviation σ of the dopant array. The concentration of the acceptor ions is set to 10^{15} cm^{-3} (circle marker), 10^{16} cm^{-3} (triangle), 10^{17} cm^{-3} (square), 10^{18} cm^{-3} (diamond). The electron concentration is set to equal (gray), 10 times as much as (solid), one-tenth (open) of the acceptor ions.

The electron mobility enhancement shown in the above results can be explained by the reduction of the Coulomb scattering. In the ordered dopant arrays, the potential energy is distributed more evenly than that of the randomly distributed ions. The Coulomb scattering probability increases as the dopant ion concentrations increases, so that the electron mobility enhancement is observed only at the higher dopant concentrations. Furthermore, when electron concentration is high enough, Coulomb scattering probability is reduced by the electron screening effect [11]. Therefore, the electron mobility enhancement appears under the condition of higher dopant and lower electron concentrations.

To measure the extent of the Coulomb scattering, we analyze the length of the trajectories of electrons. It is considered that the trajectories of electrons increase as the Coulomb scattering probability increases. Figure 5 shows the histogram of the path length of electrons while an electron goes the distance of the side length of the unit cell in the direction of

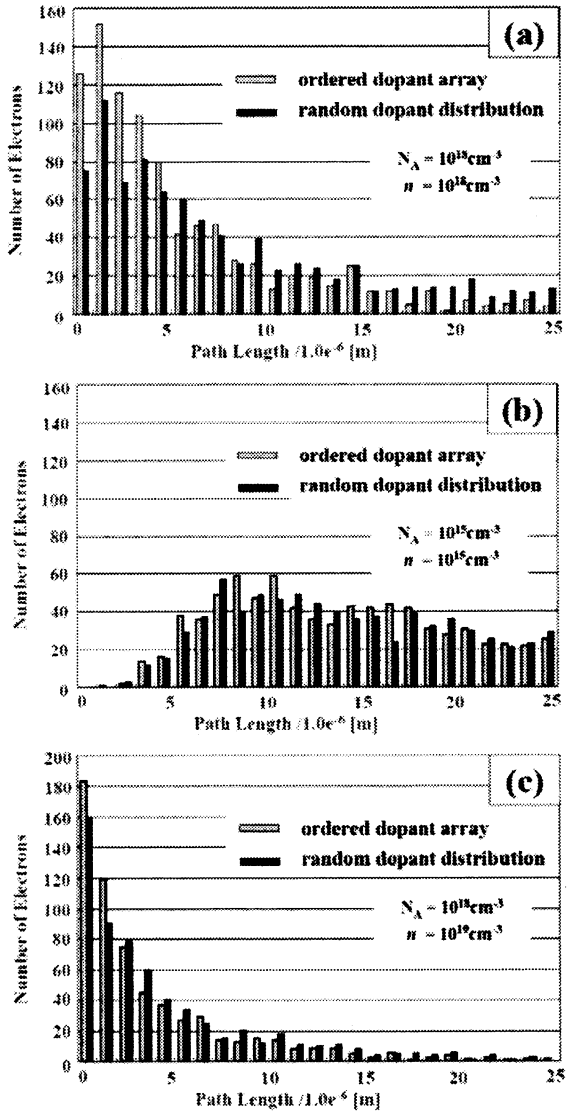

Fig.5 Histogram of the electron path length while the electron goes the distance of L (=10^{-7}m) in the direction of the electric field. (a) N_A = $10^{18}$$cm^{-3}$, n = $10^{18}$$cm^{-3}$, (b) N_A = $10^{15}$$cm^{-3}$, n = $10^{15}$$cm^{-3}$, and (c) N_A = $10^{18}$$cm^{-3}$, n = $10^{19}$$cm^{-3}$.

the electric field. Figure 5a shows the histogram obtained in the simulations of random and ordered dopant distributions under the condition of $n = N_A = 10^{18}$ cm^{-3}. At this condition, the electron mobility enhancement has been observed in the ordered arrays. The histogram in Fig. 5a shows that the number of electrons with short path lengths is larger in the ordered dopant array than in the random dopant distribution.

Figure 5b and 5c show the results obtained with the conditions of $n = N_A = 10^{15}$ cm^{-3}, and $n = 10^{19}$ cm^{-3} and $N_A = 10^{15}$cm^{-3}, respectively. In these conditions, no enhancement of the electron mobility has been observed even in the ordered dopent arrays. As shown in Fig. 5b and 5c, there is no significant difference in the histograms between ordered and random dopant distributions. Thus, the enhancement of the electron mobility in the ordered dopant arrays is attributed to the reduction in the length of the trajectories of electrons. Namely, the mobility enhancement is considered to be caused by the reduction of the Coulomb scattering probability in the uniform potential distribution of the ordered dopant array.

IV. Conclusion

We have studied the electron transport in Si with ordered dopant arrays by means of the Ensemble Monte Carlo / Molecular Dynamics simulation. Fluctuation of the dopant position from ideal ordered arrays is represented by the Gaussian distribution and we have investigated the dependency of the electron mobility on the standard deviation σ of the Gaussian distribution. The simulation has revealed that the electron mobility in the ordered dopant arrays is enhanced under the condition that the dopant concentration is higher than about 10^{17}cm^{-3} and the electron concentration is lower or equal to the dopant concentration. The enhancement of the electron mobility in the ordered dopant arrays can be attributed to the reduction in the coulomb scatterings. Present results suggest that electron mobility in a weak inversion state can be enhanced by using ordered dopant arrangement with reducing the fluctuation of position to 5 nm or smaller.

Acknowledgment

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