A Composite Ion-Implantation/Dopant Diffusion Simulation Involving Point Defect Kinetics and Its Application to Ultra Shallow Base Design

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This study proposes a unified process modeling for dopant diffusion in silicon based on point defect kinetics, and demonstrates a newly developed simulator which can predict point defect behavior from the ion-implantation process to the dopant diffusion process. This simulation has revealed the point defect induced enhancement effect on dopant diffusion during short time annealing after ion-implantation, and has accurately predicted the electric field effect in double diffusion of boron and arsenic by solving the Poisson's equation. Furthermore, triple element diffusion of boron, arsenic, and phosphorus, necessary for shallow base design in bipolar device fabrication, was successfully predicted.

1. INTRODUCTION

Accurate modeling of dopant diffusion in a silicon substrate, especially applicable to a low temperature process, is indispensable for future device fabrication. This modeling requires knowledge about the enhanced diffusion phenomenon during short time annealing after the ion-implantation process, the clustering phenomenon, double diffusion, phosphorus diffusion in high concentration, and oxidation enhanced/retarded diffusion. As decrease in the process temperature continues, modeling of the initial diffusion induced by ion-implantation damage will predominate the diffusion phenomena, since the role of the conventional diffusion mechanism will be relatively reduced.

In this work, a unified process modeling of dopant diffusion in silicon based on point defect kinetics is proposed, which can treat these phenomena simultaneously. Furthermore, a newly developed simulator, which can predict point defect behavior from the ion-implantation process to the dopant diffusion process, is also presented. Here, ionimplantation has been treated by a particle model, and point defect profiles have been obtained involving cascade generation by secondary scattered atoms. The diffusion modeling features diffusion equations for point defects involving the recombination reaction in silicon bulk under a non-equilibrium condition, and the Poisson's equation to solve the electric field effect accurately. Based on these modelings, the newly developed program was applied to the three cases of dopant diffusion during short time annealing at low temperature, double diffusion of boron and arsenic, and triple element diffusion of boron, arsenic, and phosphorus.

2. MODELING

The simulation program tool utilized in this work was composed mainly of an "ion-implantation simulator based on the particle model" and a "dopant diffusion simulator based on point defect kinetics". As shown in Fig.1, these two simulators can be operated either independently or combined through data files including dopant concentration profiles and point defect concentration profiles.

The calculation procedure in the ionimplantation simulator follows the tracing of charged particle penetration into solids.¹⁾ When the incident particle energy is neither too low nor too high, the nuclear collision process between incident ions and target atoms is approximated by successive binary collision processes. The effect of inelastic scattering



Fig.1 Schematic illustration of newly developed simulator

is modeled as energy-dependent stopping power by the Lindhard-Scharff approximation for the low energy region,²⁾ and by the Bethe-Bloch approximation for the high-energy region. The point defect concentration can be calculated taking into account the cascade generation by secondary scattered target atoms in the substrate. The target atoms recoil at energy E sufficiently larger than the threshold energy E_{th} , and the atom moves with kinetic energy $E - E_b$, where E_b is the binding energy of the atom. Here, E_{th} is assumed to take the widely used value of 15.8 eV, and E_b is assumed to be 5 eV, nearly equal to the formation energy of the Si self-interstitial.

In the dopant diffusion simulator, both the dopant concentration profiles and the point defect concentration profiles, obtained through the ionimplantation simulator, are used as the initial values. The diffusion equations for dopants and point defects are solved through the interaction of these point defects. These equations for interstitials and vacancies are given by

$$\begin{split} \frac{\partial C_{I}}{\partial t} &= D_{I} \frac{\partial^{2} C_{I}}{\partial x^{2}} - k_{R} \left(C_{V} C_{I} - C_{V}^{eq} C_{I}^{eq} \right) ,\\ \frac{\partial C_{V}}{\partial t} &= D_{V} \frac{\partial^{2} C_{V}}{\partial x^{2}} - k_{R} \left(C_{V} C_{I} - C_{V}^{eq} C_{I}^{eq} \right) . \end{split}$$

where C_I and C_V are the interstitial and vacancy concentrations, respectively. D_I and D_V are the diffusion coefficients, k_R is the bulk recombination rate constant, and C^{eq} is the concentration at thermal equilibrium.

The diffusion equation for the dopant is given

by

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[D \frac{\partial N}{\partial x} \right] + \frac{qZ}{kT} \frac{\partial}{\partial x} \left[DN \frac{\partial \psi}{\partial x} \right]$$

where C and N are the chemical concentration and active concentration, respectively. ψ denotes the potential, D the diffusion coefficient, and Z the constant value of 1 or -1. Potential ψ is solved by the Poisson's equation given by

$$\frac{\mathrm{d}}{\mathrm{d}x} \left[\epsilon \, \frac{\mathrm{d}\psi}{\mathrm{d}x} \, \right] = \rho \; .$$

Clustering phenomena are taken into account for boron and arsenic. The dissociation model for phosphorus diffusion in high concentration is also involved.

The effects of point defect populations in their different charge states on the dopant diffusion coefficient have been taken into account, on the assumption that the total concentration of charged point defects is not affected by dopant concentration. The energy required to change a charge state (less than 1 eV) is much smaller than the formation energies of point defects (≈ 5 eV). Furthermore, athermal migration requires the defect charge state to change alternatively during site to site migration.^{3–4}) Therefore, the population will be, determined mostly by the difference between the Fermi level and the defect levels. The relative populations of an interstitial C_{Iy} and a vacancy C_{Vy} in a charge state Y are given by

$$C_{I_{Y}} = C_{I} \int_{E_{I_{Y/Z}}}^{E_{I_{XY}}} f(E) dx,$$
$$C_{V_{Y}} = C_{V} \int_{E_{V_{Y/Z}}}^{E_{V_{XY}}} f(E) dx.$$

where f(E) is the Fermi distribution function, $E_{I_{X/Y}}$ and $E_{V_{X/Y}}$, and $E_{I_{Y/Z}}$ and $E_{V_{Y/Z}}$ are the energy threshold levels between the charge state X and Y, and between Y and Z, respectively. The differences in point defect levels and Fermi levels are determined by the ψ value obtained from the Poisson's equation.

The dopant diffusion coefficient can be expressed as a function of the linear combination of point defect concentrations, i.e.,

 $D = D^{eq}_{i} A^{-1} (\Sigma f_{I_{Y}} C_{I_{Y}} + \Sigma f_{V_{Y}} C_{V_{Y}}) ,$

where

 $A = \Sigma f_{I_Y} C_{I_Y}^{eq} + \Sigma f_{V_Y} C_{V_Y}^{eq},$

 f_I and f_V are the "affinity" constant for the dopant.

3. RESULTS

3-1. Initial Diffusion After Ion-Implantation

The initial diffusion phenomenon after ionimplantation is inevitable for the lower temperature process. Here, analyses were carried out on the assumption that the very initial diffusion stage are approximately expressed by a constant diffusion coefficient until the implanted damaged layer recovers to a normal crystal. Figure 2 shows the asimplanted boron and point defect profiles, with an incident energy of 40 keV and a dose of 10¹⁵ cm⁻², obtained by the ion-implantation simulator. Figure 3(a) shows the simulated and experimental boron redistribution profiles after N2 annealing at 900 °C for 1 minute, 30 minutes, and 2 hours. The redistributed profiles obtained by the conventional diffusion model⁵⁾ are also added for comparison in Fig.3(a). Figure 3(b) shows the point defect profiles corresponding to Fig.3(a). As shown in Fig.3(a), by the boron redistribution profile after N2 annealing for 1 minute, a large enhancement effect at the initial annealing stage, observed in experimental data is successfully reproduced by the new model, revealing that this enhancement effect can be attributed to a large increase in point defect concentrations, as shown in Fig.3(b). However, as the diffusion time goes on, the enhancement rapidly decreases, because the point defect concentrations decrease to equilibrium values by the recombination and diffusion processes. As a result, the simulated boron profiles after annealing for 30 minutes and 2 hours agreed well with the measured profiles.



Fig.2 As-implanted boron and point defect profiles. Solid line is boron profile, and dotted lines are vacancy and Si interstitial profiles, respectively.



Fig.3(a) Redistribution profiles for boron after N_2 annealing for 1 minute, 30 minutes, and 2 hours at 900 °C. Solid lines are results simulated with the new model. Dotted lines are results simulated with the previous model. Symbols are measured results of as-implanted profile, and of profiles after annealing for 30 minutes and 2 hours.



Fig.3(b) Point defect profiles after N_2 annealing for 1 minute, 30 minutes, and 2 hours at 900 °C. Solid lines are Si interstitial profiles, and dotted lines are vacancy profiles, respectively.

3-2. Double Element Diffusion of Boron and Arsenic

Double element diffusion of boron and arsenic is a key process for bipolar device fabrication. In the simulation of double element diffusion, one of the most important items is an accurate treatment of the electric field effect, because of the strong electric field effect at the junction region. Figure 4 shows simulated and experimental profiles for as-implanted and redistributed boron and arsenic. Arsenic was implanted with an incident energy of 40 keV and a dose of 5x10¹⁵ cm⁻². Boron was implanted with an incident energy of 40 keV and a dose of 1x10¹⁵ cm⁻², successively. Annealing was carried out in N2 ambient at 900 °C for 30 minutes. The simulation result obtained by the conventional model is also shown in Fig.4. By comparing these profiles, it can be confirmed that the redistribution profiles diffusing backward at the junction region by a strong electric field are well produced by the proposed simulation.



Fig.4 Redistribution profiles for boron and arsenic after N_2 annealing for 30 minutes at 900 °C. Solid lines are results simulated with the new model, and dotted lines are results simulated with the conventional model.

3-3. Application to Shallow Base Design

Triple element diffusion of boron, arsenic, and phosphorus is efficient for shallow base design, since the base width can be controlled using fast phosphorus diffusion. However, phosphorus diffusion in high concentration largely affects boron diffusion. Dopant diffusion was simulated taking into account the increase in vacancy concentration by dissociation reaction. Figure 5 shows an example of application to shallow base design, including as-implanted profiles and redistribution profiles for three dopants. Annealing was accomplished in a N_2 ambient at 900 °C for 75 minutes. The simulated profiles agreed well with the measured profiles.

4. CONCLUSION

A unified process modeling for dopant diffusion in silicon based on point defect kinetics has been proposed. A newly developed simulation tool combining an ion-implantation simulator with a dopant diffusion simulator, has been presented. The simulation accurately predicted the enhancement effect of dopant diffusion during short time annealing at low temperature, by following point defects generated by ion-implantation, and the electric field effect of double element diffusion by solving the Poisson's equation. Furthermore, by using the phosphorus dissociation model in high concentration, the simulation allowed designing shallow base fabrication processes.



Fig. 5 Redistribution profiles for boron, arsenic, and phosphorus after N_2 annealing for 75 minutes at 900 °C.

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