Monte Carlo Impurity Diffusion Simulation Considering Charged Species

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Abstract

A Monte Carlo dopant diffusion simulation program has been developed which includes charged species, i.e. Fermi-level effects on drift-diffusion and reactions. In order to save computational time, an algorithm that determines variable time steps was improved to account for all the Fermi-level dependent quantities, such as different charge states of point-defects, pairs and complexes, and different diffusivities/reaction rates for them. Simulation of coupled arsenic and boron diffusion for a typical sub-100nm CMOS process has been demonstrated by using this MC program.

1 Introduction

Recently, several sub-50nm CMOS devices have been demonstrated [1][2]. Their extremely small features and extreme process conditions, e.g. 550℃ for 10 hour anneal or 1100℃ for spike anneal with a 300℃/s ramp-up rate, have challenged conventional process simulators.

In order to simulate such critical MOSFET characteristics, more precise impurity diffusion and activation models are required not only for accurate impurity profiles, but also for evaluating dopant distribution fluctuations which degrade some device characteristics, e.g. threshold voltage uniformity[3]. Some atomistic approaches for modeling dopant diffusion and activation kinetics have been reported over the last few years[4][5].

More recently, attempts were made to improve the predictive capability by incorporating *ab initio* calculations of the energetics of the key diffusing species in the model, e.g. boron clustering[6]. Even the full-CMOS process simulation may be feasible if such an atomistic approach could include some more practical aspects, such as more realistic boundary conditions, Fermi-level effects, and a more efficient computational task for 2-3 dimensional simulations. In this paper, a kinetic Monte Carlo diffusion simulation method is described with emphasis on these features.

2 Model

The basic model for the diffusion simulation is a random walk, where the hopping motion is off-lattice of crystal silicon, i.e. a kinetic Monte Carlo dopant diffusion simulation similar to DADOS[7] code.

Every jump and reaction event is calculated with the discretized variable time step which is determined as the inverse of the sum of every event frequency[7]. Our code considers more than one dopant atom, point defects, pairs, clusters and complexes. Ion implantation is simulated also by a separate MC code[8].

$I^- I^0 I^+, I^{++}, V = V^- V^0 V^+,$
$B^- BI^- BI^0, BI^+,$
$As^+ AsV^+ AsV^0 AsV^-, As_2V^0, ...$

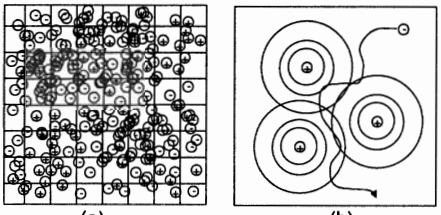

Figure 1: Typical charged species considered in the model. Electrostatic potential is represented by (a) grid based Poisson equation, or (b) screened Coulomb potential.

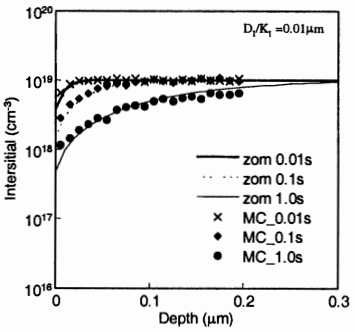

Figure 2: Calculation results for initially flat excess interstitial-Si diffusion behavior assuming finite surface recombination rate(K_I). Comparison is made to the continuum model solutions(solid lins).

Here, we have tested two features, one is the incorporation of all the charged-species, and the other is finite recombination rates for the point defects at the interface. Each substitutional dopant atom has its specific charge state. Monte Carlo particles represent the total number of point defects and pairs in the model, but the charge states are considered every time when they jump or react with other species according to the local electrostatic potential.

The local potential is determined by solving the Poisson equation on a discretized grid (Fig.1(a)) with Newton iteration, since the population of charged point-defects that is determined by the local Fermi-level. In most cases, however, the quasi-neutral approximation is applied instead of solving Poisson equation. The grid-based representation of the local potential implies some artificial averaging of potential fluctuations but these can be captured by considering individual screened Coulomb potentials from the charged species (Fig.1(b)). However, this grid-based representation is also useful for the efficient calculation of the variable time steps. Evaluation of the event is the most computationally intensive step, especially when the model includes disparate different diffusivities or reaction rates for each species.

The computational cost for re-calculation of the specific event frequency was significantly reduced by evaluating the local event or local potential only for the grid element where the particle population was changed. This method enables us to simulate practical process conditions.

All the boundary conditions are set to be periodic or mirror except for the interface and the bottom. The interface is not a perfect sink for point defects but can be described by the finite recombination length $D_I/K_I \simeq 0.01 \sim 0.1\mu m$[9]. This boundary condition was successfully incorporated in our code (Fig.2).

3 Results and discussion

Almost all of the physical parameters in the model are taken from the literature, but some of them were modified slightly to account for the finite K_I and charge states assumed in this model.

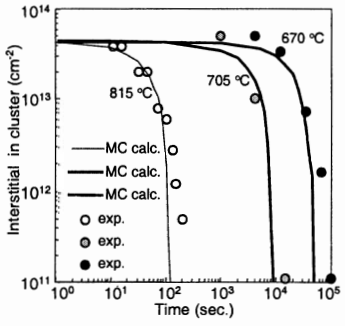

Figure 3: Calculation results for the {311} interstitial cluster dissolution. Experimental data are taken from [10].

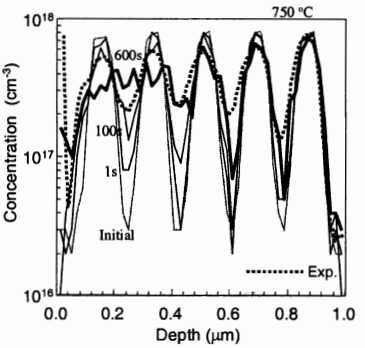

Figure 4: Calculation results compared with the data from the delta-doped boron markers with 40keV 5e13cm^{-2} Si implantation and annealing experiment[11].

The point defect cluster kinetics (Fig.3) and boron transient enhanced diffusion (Fig.4) can be reproduced by the single set of the parameters. Using this MC code, a coupled arsenic and boron diffusion was calculated considering typical process conditions for sub-100nm CMOS. The arsenic source/drain is not only shallow but also includes a high arsenic concentration surrounded by over $10^{18}cm^{-3}$ substrate boron doping(Fig.5). Boron redistribution occurs during the annealing due to the charged species population difference near the PN junction and the electric field effects. The MC calculation was done in a 3D computational cell of $0.1(L) \times 0.5(Depth) \times 0.2(W)[\mu m]$. The results are shown in 1D (Fig.6) and 2D (Fig.7 and Fig.8). A typical CPU-time for the annealing calculation is about 21 hours on a DEC-α 500MHz workstation.

The result shows boron pile-up in the high concentration arsenic source/drain region (Fig.6) and the resulting depletion near the source/drain (Fig.7) which would change the short channel effect.

Analyses of this Monte Carlo simulation results show that the boron redistribution is

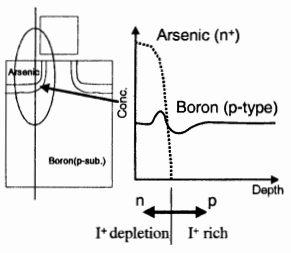

Figure 5: Schematic representation of the redistribution of the substrate boron near the arsenic source/drain.

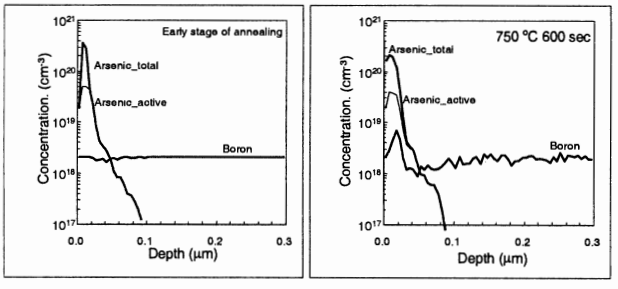

Figure 6: Calculation results for coupled arsenic and boron diffusion. Boron concentration was initially flat. Arsenic was implanted at 10keV, $5e14cm^{-2}$. Calculation region is $0.1(L) \times 0.5(Depth) \times 0.2(W)\mu m$.

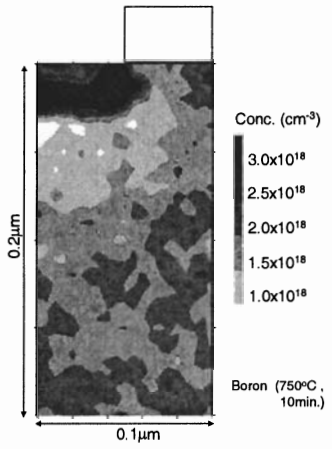

Figure 7: Two-dimensional contour representation of the calculation result for boron shown in Fig.6. (Concentrations were averaged over the W-direction.)

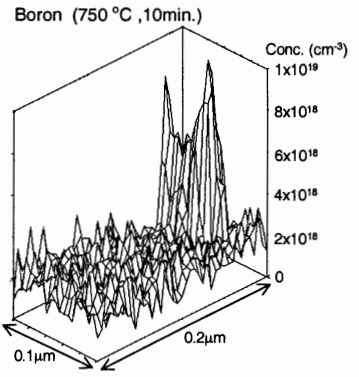

Figure 8: Same as Fig.7 but with boron concentration plotted on the vertical axis.

mostly caused by the population difference of BI pairs in different charge states between the highly doped n^+type region and the p^-type substrate region.

4 Summary

The Monte Carlo diffusion (and implantation) simulator described here has been shown to be suitable for application to sub-100nm CMOS, where the extremely small features require advanced, physically correct (atomic-level) models. Such models can incorporated in our MC code, and simulations of actual process conditions can be accomplished in a reasonable amount of computer time.

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