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Calibration of TCAD Models for High Dose Impurity Diffusion

Osamu Nishio, Masahiro Takenaka, Eiji Aoki, Norio Mizukoshi and Katsumasa Fujii
VLSI Development Laboratories, SHARP Corporation, Ichinomoto-cho, Tenri-shi, Nara 632, Japan
Phone: +81-7436-5-4856, Fax: +81-7436-5-2774, E-mail: nishio@icg.sharp.co.jp

1. Introduction

It is well known that the dopant - defects pair diffusion model fails to estimate high concentration impurity diffusion in Si. So far the simulation overestimates the diffusion of high concentration impurities. This problem must be overcome to make TCAD tools predictable.

As a cause of suppression of TED (Transient Enhanced Diffusion), it is said that dislocation loops [1] or {311} defects [2] absorb excess interstitial Si generated during ion implantation, and they gradually dissociate the interstitial Si during annealling. Further, Morehead et. al. assume that excess interstitial Si make dopants immobile clusters before they absorbed into dislocation loops or {311} defects [3] (transient clustering model) .

In this work, the dopant clustering models (transient clustering model and equilibrium clustering model) for boron and arsenic diffusion in both the furnace anneal and the RTA are calibrated and TSUPREM-4 simulation results are compared with SIMS profiles. Further RSCH (Reverse Short Channel Effects) simulation results from MEDICI are compared with experimental data.

2. Models and Calibration

Defects generation at Ion Implantation

Basically the "+1" damage model [4] and the Frenkel pair model are used. It is considered that the Frenkel pair disappear by interstitial Si - vacancy recombination in bulk Si at the start of the anneal. Since the surface recombination rate of interstitial Si and vacancy is different, Interstitial Si and vacancy concentration are not the same at the Si/SiO_2 interface and this affects diffusion.

When the source/drain is ion implanted (high dose), Frenkel pair generation is limited under amorphizing threshold level. In this case, interstitial Si and vacancy concentrations are equal near the surface. However, a difference between interstitial Si and vacancy concentrations at the Si/SiO_2 interface occurs after the anneal starts.

Transient Clustering Model [5]

The transient clustering is divided into two phases. In the first phase impurity forms into clusters assisted by implantation induced interstitial Si [6]. In the second phase the impurity cluster dissociates impurity atoms during the anneal. The clustering of impurity in the first phase occurs very fast so even RTA is longer enough than the clustering time. Therefore the first phase is not included in this simulation. The clustering rate is determined as an initial value for the second phase. In the declustering phase dissociated dopant atoms increase from the initial active concentration to equilibrium active concentration. The declustering rate at each time step is calculated by a time constant τ which depends exponentially on the anneal temperature.

In our calibration, τ for boron shows the values, 660sec at 850°C and 0.3sec at 1000°C.

Equilibrium Clustering Model

Equilibrium active concentration of boron is so far determined by solid solubility which depends on only temperature. The clustering model for boron as well as for arsenic is used. In this model, the equilibrium active concentration of boron depends on anneal temperature and chemical concentration.

3. Calibrated Results

High Dose Boron Profile

The comparison between simulation results and experimental (SIMS) data after anneals are shown in Fig.1. In each case, ion implantation has 2 steps ((1) dose : 3E13 atoms/cm^2, energy : 20 keV, (2) dose : 2E15 atoms/cm^2, energy : 10 keV). Fig.1(a) and (b) shows profiles after 850°C 30min furnace anneal and after 1000°C 10sec RTA, respectively.

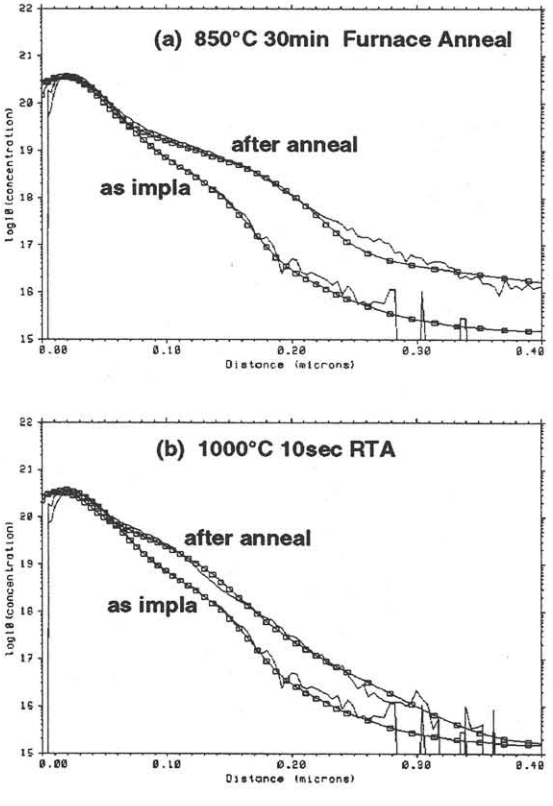

Fig.1 Boron profile after anneal (line : SIMS data , symbol : simulation) . As-impla profile is fitted to SIMS data .

High Dose Arsenic Profile

Simulation of source/drain region with experiment (SIMS) data is shown in Fig.2. Simulation results without (Fig.2(a)) or with (Fig.2(b)) transient clustering model are also compared to SIMS profiles. In this case, the transient activation model is applied to high dose arsenic (implant dose : 3E15 atoms/cm^2, energy : 50 keV). Simulation results of other species (boron, phosphorus) are also improved, and simulation results agreed with the experimental data except for the phosphorus profile in the vicinity of the interface.

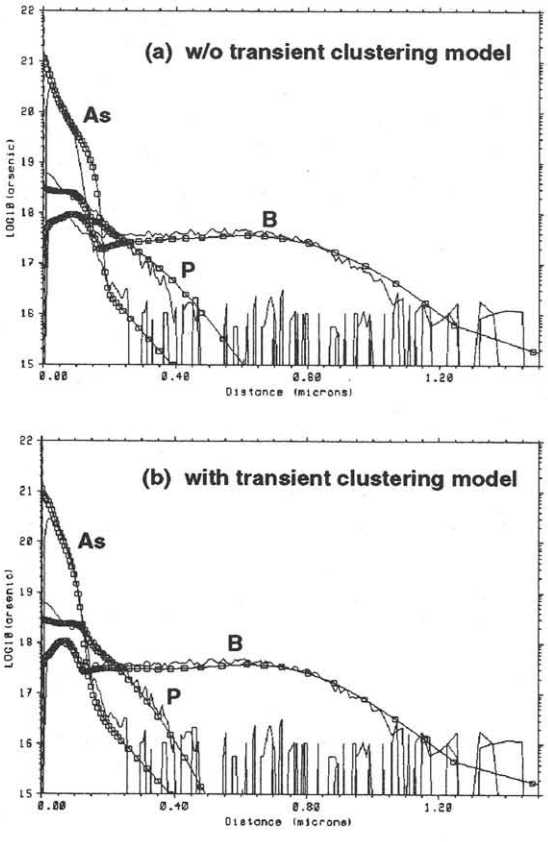

Fig.2 Impurity profiles after anneal at NMOS source/drain region (line : SIMS data , symbol : simulation).

Reverse Short Channel Effect

Boron for punch through stop, Vth adjust, and p-well formation and interstitial Si generated by source/drain implantation makes dopant - defects pair and diffuses in excess rate. The recombination rate of interstitial Si at the interface is much higher than the rate in bulk Si so boron decoupled from interstitial Si remains and accumulates at the interface.

The accumulation of boron causes Reverse Short Channel Effects on NMOS transistors. By calibration of recombination rates at interface and bulk, the accuracy of the simulation is much improved. Simulation of RSCE is shown in Fig.3. In Fig.3(a), simulation results of 3 different Halo (punch through stop) implantation energies are compared to experiment data in each case. In Fig.3(b), simulation results of 3 different Halo implantation doses are compared to experimental data in each case.

The recombination rates in this simulations are,
9.9E+1 cm/sec (interstitial Si at surface, 850°C)
2.8E-3 cm/sec (vacancy at surface, 850°C)
3.1E-17 cm^3/sec (in bulk Si, 850°C).

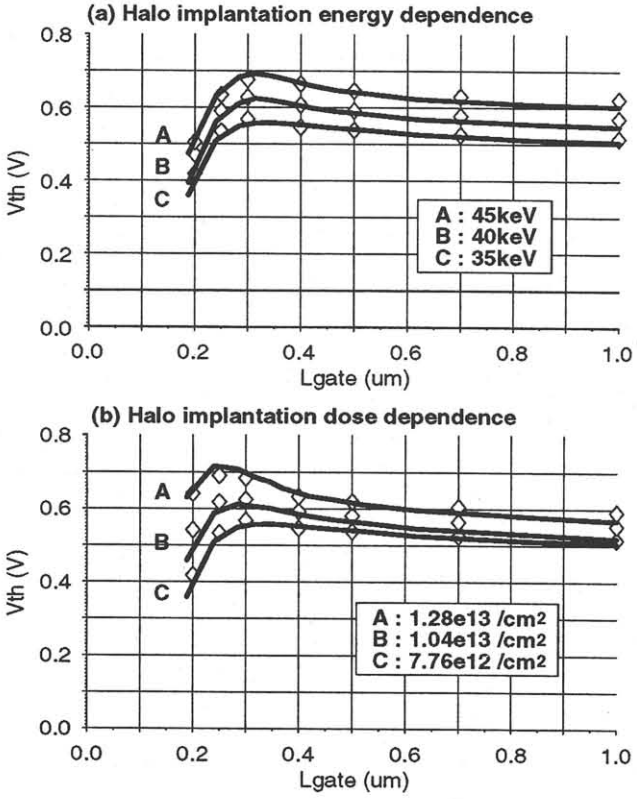

Fig.3 Vth vs. Lgate (line : measurement , symbol : simulation).

4. Conclusions

It is shown that the accuracy of process simulation is much improved by using the transient clustering, equilibrium clustering and TED models.

By performing calibration, the declustering rate in the transient clustering model is obtained.

As a result, we can estimate the effects during rise time and fall time of temperature at RTA and furnace anneal.

Through the calibration of RSCE, the recombination rate at the surface and the rate in bulk Si are estimated.

Through this calibration, it becomes clearer that modification of the TED model such as transient clustering much improves the accuracy of not only process simulations but also device simulations and increase the predictability of the TCAD tools.

References

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