Edited by H. Ryssel, P. Pichler - September 1995

Precipitation phenomena and transient diffusion/activation during high concentration boron annealing

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Abstract

The understanding of low thermal budget transient diffusion and activation of shallow p^+ implants remains a crucial issue of technology simulation. In this paper, we apply a coupled point defect assisted diffusion/precipitation model to the redistribution phenomena observed during annealing of shallow boron implants. Comparison with experimental data shows that the precipitation model can account for unusual segregation phenomena in the highly disordered zone around the projected range of the as–implanted profile.

1. Introduction

The complexity of high concentration boron activation and transient enhanced diffusion (TED) has challenged the process modeling community for some years now [1, 2]. The trend towards low thermal budget and the inevitability of boron as a high dose p-dopant in e.g. PMOS transistor fabrication requires development and calibration of process simulation tools which mirror the physical processes involved. As far as TED phenomena are concerned, point defect assisted diffusion models have proved to be the most powerful approaches, because unlike empirical models they give a more consistent view of nonlocal diffusion effects. In the framework of sophisticated point defect models, TED is usually modeled making assumptions on the initial point defect supersaturation present in the crystal immediately after implantation. Dopant activation phenomena have been described in terms of nonequilibrium cluster models [3], or, most recently, by applying precipitation models to laser activated arsenic and phosphorus square profiles [4].

In our contribution, we will present the application of a nonequilibrium point defect/dopant precipitation model to the redistribution and activation of high–dose, inhomogeneous boron profiles during rapid thermal anneals (RTA) and furnace anneals.

The activation of boron is modeled by tracing the dynamics of a spatial dependent size distribution of boron clusters.

2. Model description

In particular, we solve a coupled drift–diffusion–reaction system, covering balance equations for interstitials, vacancies and dopants in various charge states. The fluxes $\mathbf{j}$ of dopant-interstitial pairs $(A_jI)^{(z)}$ and isolated interstitials I^z read

$$\mathbf{j}_{(A_jI)^{(z)}} = -D_{jIz}k_{jIz}\left(\frac{n}{n_i}\right)^{(-q_j-z)} \nabla\left[C_{A_j^{(q_j)}}C_{I^0}\left(\frac{n}{n_i}\right)^{(q_j)}\right] \tag{1}$$

and

$$\mathbf{j}_{I^{(z)}} = -D_{Iz}k_{Iz}\left(\frac{n}{n_i}\right)^{(-z)} \nabla C_{I^0}, \tag{2}$$

respectively, where C_X, D_X, n, n_i, k_{jIz} and k_{Iz} denote the concentration of species X, diffusivity of species X, electron density, intrinsic carrier density, equilibrium constants for interstitial and pair ionization, respectively. Exponents in parentheses denote charge states. Similar fluxes are used for vacancies and dopant–vacancy pairs.

For the precipitates, we solve a coupled reaction system at every gridpoint. Assuming charge conservation, the growth rate $R_{N\to N+1}$ of precipitates containing N boron atoms is

$$R_{N\to N+1} = k_f^N\left[C_NC_1\left(\frac{n}{n_i}\right)^q - k_{eq}^NC_{N+1}\right], \tag{3}$$

where C_N, C_{N+1}, C_1, n and n_i denote the concentration of precipitates of size N, size $N+1$, isolated dopants (q-fold charged), electrons and intrinsic electron density, respectively, and k_f^N is the reaction rate. The reaction system of precipitates is written as

$$\frac{\partial C_N}{\partial t} = -R_{N\to N+1} + R_{N-1\to N} \qquad 1 < N < N_{max} \tag{4}$$

$$\frac{\partial C_N}{\partial t} = R_{N-1\to N} \qquad N = N_{max} \tag{5}$$

$$\frac{\partial C_1}{\partial t} = -\nabla\mathbf{j}_1 - R_{1\to 2} - \sum_{N=1}^{N_{max}-1} R_{N\to N+1} \qquad N = 1, \tag{6}$$

where $\mathbf{j}_1$ denotes the flux of the particles of "size 1", which is a sum of fluxes of the type Eq. 1. The equilibrium constant k_{eq}^N is determined by the Gibbs–Thomson equation:

$$k_{eq}^N = \Theta\frac{C_L}{C_P}C_{sol}\exp\left(\frac{\Delta G_N}{k_BT}\right), \tag{7}$$

where C_L, C_P and C_{sol} are the concentrations of silicon lattice sites, boron atoms in a precipitate, and equilibrium boron solid solubility, respectively. ΔG_N is the size dependent excess free energy change due to the particle transition from the surrounding matrix to the precipitated phase. The factor Θ accounts for possible degeneracies.

The simulations are carried out with the latest version of TESIM [5], a one–dimensional multilayer process simulator.

3. Model assumptions

A modified "+1"–model is used as the initial damage assumption, which means that the interstitial distribution in the beginning of the simulation follows the as–implanted doping profile. We use an equilibrium clustering model for interstitials, to obtain the experimentally observed TED. Recently, small dissolving {113} stacking faults have been experimentally identified as the interstitial source at the intial stage of implantation/annealing steps, giving evidence to the interstitial cluster picture [6]. We started the simulations with a completely inactive profile, and a nuclei size distribution which corresponds to the local total as–implanted boron concentration. A concentration dependent nuclei size distribution above a certain nucleation threshold is given as a tentative explanation for unusual "up–hill" diffusion phenomena observed in the heavily disordered region around the projected range of implanted ions.

4. Results

Fig. 1 shows a comparison of experimental and calculated results of a 10s, 1000°C boron RTA experiment, with implantation conditions as shown in the insert. The RTA simulations included measured temperature ramps. The transient diffusion model works quite satisfactory, as can be seen from the diffusion tail. Fig. 2 illustrates the situation at 900°C during the ramp–up.

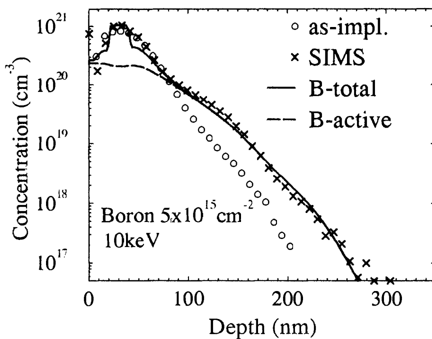

Figure 1: Comparison of experimental and simulated (lines) profiles of a 10s, 1000°C boron RTA experiment.

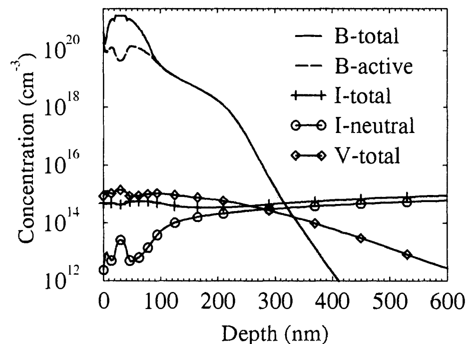

Figure 2: Simulated dopant and point defect concentrations during ramp–up.

The SIMS profile suggests an "up–hill" diffusion at the peak of the profile, which is reproduced by the simulation. From the simulation point of view, the reason is that large, slow–dissolving or even growing precipitates are present in this region, which acts as a boron sink. Figs. 3 and 4 show the spatial dependence of the distribution function during the ramp–up at 900°C, and after the complete thermal cycle, respectively. One can observe a dip in the active concentration (precipitates of "size 1") during ramp–up, which leads to the increase of the total concentration.

5. Conclusion

Transient enhanced diffusion and activation of shallow boron implants has been studied using a coupled pair diffusion/precipitation model. TED was described using a

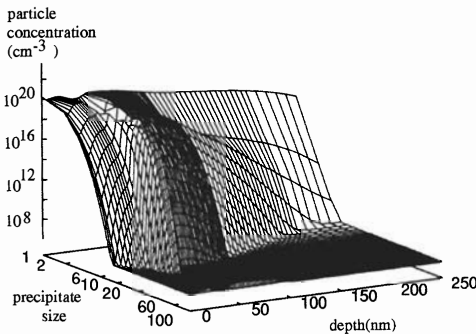

Figure 3: Spatial distribution of boron precipitates during ramp up at 900°C.

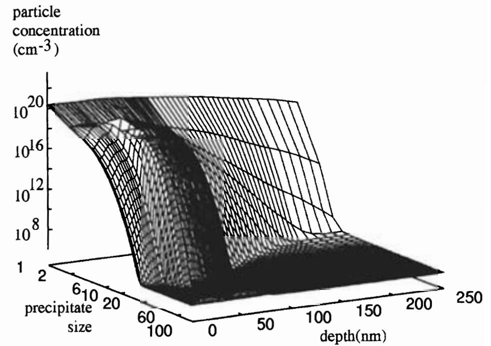

Figure 4: Spatial distribution of boron precipitates after the full RTA temperature cycle.

modified "+1"-model. Activation could be modeled successfully taking advantage of the time development of a spatially dependent size distribution function of boron precipitates.

6. Acknowledgements

This work was supported by the swiss priority program on power electronics, systems and information technology (LESIT) and Cray Research, Inc.

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