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Modeling Boron Profiles in Silicon after Pulsed Excimer Laser Annealing

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Abstract. In this work, we investigated four possible mechanisms which were candidates to explain the shape of boron profiles after ion implantation and melting excimer laser annealing in silicon. A laser with a wavelength of 308 nm and a pulse duration of ~ 180 ns was used. To simulate this process, an existing model for the temperature and phase evolution was complemented with equations for the migration of dopants. Outdiffusion, thermodiffusion, segregation, and adsorption were investigated as possible mechanisms. As a result, we found that outdiffusion and segregation can be excluded as major mechanisms. Thermodiffusion as well as adsorption could both reproduce the build-up at low melt depths, but only adsorption the one at deeper melt depths. In both cases, ion beam mixing during SIMS measurement had to be taken into account to reproduce the measured profiles.

Keywords: Laser thermal annealing, silicon, simulation, boron, adsorption, ion-beam mixing

PACS: 61.72.U-, 64.70.kg, 61.20.Ja

INTRODUCTION

Pulsed excimer Laser Thermal Annealing (LTA) is a process that allows dopant activation and damage removal of ion implanted samples. The low thermal budget of a laser pulse with pulse duration in the nanosecond regime allows melting and recrystallization (liquid phase epitaxy) of the implanted region while no significant annealing of areas away from the surface [1] takes place. This can, for example, be used for shallow junction formation [2] and 3D integration [3].

Boron redistribution in silicon during LTA was investigated by Monakhov et al. [4] using a 308 nm XeCl excimer laser with a pulse duration of 28 ns and by Ong et al. [5] using a 248 nm KrF excimer laser with a pulse duration of 23 ns. In both investigations, the boron profiles in silicon show a depletion near the sample surface and a build-up at the initial liquid/solid interface in silicon. This shape cannot be explained by simple Fickian diffusion since this would imply diffusion against the concentration gradient.

To explain the build-up of boron, Monakhov et al. [4] suggested the formation of B-Si clusters. However, the authors themselves noted that the build-up doesn't scale with dose according to a power law as expected for a clustering phenomenon. In addition, no reduction of the boron diffusivity was observed during

subsequent heat treatments which indicates that the boron atoms were electrically active.

Ong et al. [5] conducted an experiment which is particularly relevant for model development. After a first laser shot with a high energy density, resulting in a nearly flat dopant profile, they annealed the sample for a second time with the maximum melt depth located in the flat region. They explained their observed build-up with the following model: After reaching the maximum melt depth, recrystallization starts with a bulk segregation coefficient k of less than unity. Defined as ratio of the concentrations in the solid and liquid phases, a bulk segregation coefficient of less than unity leads to a build-up of dopants in the liquid. With increasing melt-front velocity, k increases to unity and even slightly beyond, causing a gradual decrease of the concentration. Towards the surface, k is suggested to decrease to unity again.

However, such assumptions would not reproduce the measured profile around the maximum melt depth. For a bulk segregation coefficient of less than unity, a smaller concentration of dopants than in the liquid is incorporated into the newly grown solid layer. Based on an initially homogeneous concentration on both sides of the melt interface, one expects a drop of the concentration in the regrown layer before the concentration finally increases. However, this drop was not observed experimentally.

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As the understanding of the build-up formation and the prediction of the doping profiles by simulation is important for an effective support of device design by Technology Computer Aided Design (TCAD), we investigated possible mechanisms for depletion and build-up.

EXPERIMENTAL PROCEDURE

To investigate the build-up, we used silicon samples that have been ion implanted with an energy of 3 keV and a dose of $3 \times 10^{13} \text{ cm}^{-2}$. The samples were then annealed with single laser pulses with energy densities (E_{las}) of 1.95 J/cm², 2.05 J/cm², and 2.35 J/cm². The laser used was a XeCl excimer laser with a wavelength of 308 nm and pulse duration of 180 ns. The resulting profiles shown in Fig. 1 where measured by SIMS using a 1 keV O₂ beam impinging with an angle of 44°. As in the previous investigations [4,5], the profile shape is characterized by a build-up of boron near the melt depth and a depletion at the surface. This indicates that the different wave lengths and pulse durations of the experiments cannot be dominating factors.

FIGURE 1. Measured boron profiles after LTA.

SIMULATION RESULTS AND CRITICAL DISCUSSION

As the mechanisms proposed in the literature to explain the shape of the boron profiles after LTA are not able to fully explain the experiments, we explored alternative explanations. To simulate dopant redistribution, we used an enthalpy-based model for the temperature and phase evolution during melting laser annealing [6], extended it with different mechanisms for mass transport, and implemented it in Sentaurus Process of Synopsys [7].

One important factor for simulating the diffusion of dopants in the liquid is the respective diffusion coefficient. Based on the work of Garandet [8] and

Tang et al. [9] we assumed that its value should be somewhere between $1.6 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ and $2.5 \times 10^{-4} \text{ cm}^2 \text{ s}^{-1}$. In this range, we used it as a fitting parameter.

Outdiffusion: One mechanism that could be responsible for the dopant depletion towards the surface is outdiffusion of dopants from the liquid phase to the gas or covering SiO₂ layers. We modeled this effect by a continuity equation in the form

$$\frac{dC_B}{dt} = \nabla(D_B \nabla(C_B)) - s(x)k_{\text{out}}C_B \quad (1)$$

with the first term on the right-hand side to account for dopant redistribution by Fickian diffusion. C_B and D_B denote the concentration and diffusion coefficient of boron, respectively. In the solid silicon phase, a vanishing diffusion coefficient is assumed. This approximation is reasonable since, due to the comparatively small diffusion coefficient in the solid phase, no noticeable dopant redistribution is expected there during our simulation time of 500 ns. The second term on the right-hand side describes the outdiffusion at the surface. k_{out} stands for the respective outdiffusion coefficient. $s(x)$ is unity for the cells at the surface and zero elsewhere. The profiles are then determined by the product of k_{out} and the grid spacing at the surface which was 5 nm in our simulation.

Figure 2 shows the results of the simulations with the lower limit of the diffusion coefficient of $1.6 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ in the liquid phase and the outdiffusion coefficient varied between 0 and $5 \times 10^8 \text{ s}^{-1}$. For clarity, only simulations for the deepest melt case ($E_{\text{las}} = 2.35 \text{ J/cm}^2$) are compared with the corresponding SIMS result. This highest laser energy density was chosen as it leads to the longest melt duration and the highest amount of outdiffused dopant atoms.

FIGURE 2. Simulated outdiffusion profiles in comparison with the SIMS measurement.

The simulations show that in order to obtain a depletion comparable to what was measured near the surface, the outdiffusion coefficient has to be around

$\sim 5 \times 10^8 \text{ s}^{-1}$. But for such a case, the simulated dose loss would be much too high in comparison to the experiment. Higher diffusion coefficients in the liquid phase would even lead to an increased dose loss for the same gradient at the surface. Therefore, simple outdiffusion can be ruled out as major mechanism responsible for the shape of boron profiles after excimer laser annealing.

Thermomdiffusion: One effect that could explain the apparent dopant migration from the surface towards the melt front is the assumption of a temperature gradient as driving force. In analogy to diffusion in a concentration gradient, this effect is referred to as thermomdiffusion or Soret effect. In liquid silicon, thermomdiffusion was investigated e.g. by Eslamian et al. [10] during zone melting with aluminum as dopant. Unfortunately, a predictive theory for the thermomdiffusion coefficient in liquids is still not available [11].

To include the effect of a temperature gradient, we used a continuity equation in the form

$$\frac{dC_B}{dt} = \nabla(D_B \nabla(C_B)) + \nabla(D_T C_B \nabla(T)) \quad (2)$$

with T denoting the temperature and D_T the thermomdiffusion coefficient. Again, the first term on the right-hand side describes Fickian diffusion. As the value D_T for boron in liquid silicon is unknown, it was used as a fitting parameter.

FIGURE 3. Simulated profiles using the thermomdiffusion equation and convolved profiles compared to the SIMS measurement.

Figure 3 shows the best fit with $D_T = 9.25 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1} \text{ K}^{-1}$ and $D_B = 7.6 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$. The overall trends of the SIMS measurement can be reproduced. However, compared to the SIMS measurements, the drop in concentration at the maximum melt depth is too steep and the depletion at the surface is not reproduced.

SIMS correction: The discrepancy in steepness of the measured and simulated profiles could be an artifact of the SIMS measurement. During SIMS measurement, primary ions are used to sputter target ions out of the sample to be analyzed. Target atoms hit by a primary ion which are not sputtered can be pushed deeper into the sample. This effect is called ion-beam mixing and expected to be a major source of profile distortion in our case. To take the effect into account, we used a method developed by Saggio et al. [12]. In a first step, we used our in-house Monte-Carlo simulator MCSIMS to calculate the SIMS response of a boron δ -layer by the binary collision approximation. The result is shown in Fig. 4. The SIMS δ -response function was then convolved with the dopant profile to obtain the result SIMS would show if ion-beam mixing were the only source of profile distortion.

FIGURE 4. Simulated SIMS signal of a boron δ -layer for a 1 keV O_2 beam impinging with an angle of 44° .

The result of the convolution of the simulated profiles using the thermomdiffusion model with the SIMS δ -response function is shown also in Fig. 3. Now, it can be seen that the steepness of the measured profiles and the simulated profiles are similar for the high and medium melt depth cases. For the profile with the smallest melt depth, other sources of profile distortion could also affect measurement accuracy. Surface roughness, for example, could further limit the capability of SIMS to measure steep profiles.

Within the first few nanometers, the simple profile convolution is not expected to be reliable. Therefore, the slight drop in concentration apparent in the convolved profiles at the surface is considered an artifact of the method.

Adsorption: As thermomdiffusion did not allow us to simulate the experimental profiles sufficiently well, adsorption of dopants at the solid-liquid interface, also called interface segregation, was considered. The diffusion-segregation equation developed by You et al. [13]

$$\frac{dC_B}{dt} = \nabla(D_B \nabla(C_B)) - \nabla(D_B \frac{C_B}{C_{equ}} \nabla(C_{equ})) \quad (3)$$

was used for this purpose. As before, the first term on the right-hand side describes Fickian diffusion. The second term is used to describe the segregation of the boron atoms. In steady state, the concentration in the vicinity of the interface is proportional to the equilibrium concentration C_{equ} and the right-hand term vanishes. The equilibrium concentration used in each phase is shown in Fig. 5.

FIGURE 5. Shape of the equilibrium concentration used for the simulation of adsorption.

It is apparent from (3) that a multiplication of C_{equ} with a non-vanishing constant does not change the result. Without loss of generality, we set C_{equ} to unity in the liquid. In the solid, C_{equ} corresponds then to the equilibrium segregation coefficient for which we adopt a value of 0.8 from the work of Trumbore [14]. In the interface region between the liquid and solid, a value higher than unity is assumed to simulate adsorption. The width of the interface is one grid point in our simulation.

The results of this simulation together with the convolved profiles are shown in Fig. 6.

FIGURE 6. Simulated profiles using the adsorption model and convolved profiles compared to the SIMS measurement.

Assuming adsorption, the pile-up of dopants near the maximum melt depth as well as the depletion at the surface could be reproduced well. Taking ion-beam mixing into account results in a further improved agreement between simulation and experiments.

The best fit resulted in a diffusion coefficient of $2.4 \times 10^{-4} \text{ cm}^2 \text{ s}^{-1}$ in the liquid. For the interface region, a segregation coefficient of 2.8 and a diffusion

coefficient of $1.8 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$ were obtained. The value of the diffusivity in the interface limits the capability of the adsorbed layer to keep up with the moving interface. This means that at low velocities, the expected segregation value of 0.8 can be observed while with increasing velocity, more and more dopants are trapped in the newly grown solid layer during recrystallization.

A comparison of the results from the adsorption and thermodiffusion models shows that the adsorption model reproduces the build-up more accurately. This is especially visible in the medium melt depth case. For the dopant tail in the lowest melt depth case, the same arguments as in the thermodiffusion case apply.

CONCLUSIONS

We have investigated several models to explain boron redistribution after LTA. Comparisons between simulations and experiments allowed ruling out outdiffusion as a major mechanism. The pile-up predicted by the thermodiffusion model drops much faster with the maximum melt depth than in the experiments and also fails to explain the depletion at the surface. Among the approaches considered, only the adsorption model allows the correct reproduction of experimental profiles for all three laser energy densities, provided that the profile distortions induced by SIMS are taken into account in the simulations.

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