Simulation of low energy ion implantation in silicon

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Abstract. This report is devoted to simulation of distributions of boron and indium ions implanted into the silicon substrates with energies up to 10 keV. The simulation was conducted immediately after implantation and after subsequent annealing in inert and oxidizing ambient. Post-implant and post-anneal distributions of impurities concentration versus depth were obtained. It was demonstrated, that the super-steep retrograde distribution of indium in silicon is provided exactly by the annealing in an oxidizing ambient. Also, it was demonstrated, that the annealing does not provide the super-steep retrograde distribution of boron in silicon. Thus, it was shown, that indium doping of gate region contributes to suppression of the short-channel effects in nanoscale MOSFETs, unlike boron doping.

1. Introduction

Doping of the gate region applies to the threshold voltage control of MOSFETs. For this purpose, boron doping is widely used at manufacturing of microscale transistors. But this impurity does not suppress the short-channel effects of nanoscale transistors. Recently, indium doping of the gate region is increasingly used at manufacturing of the nanoscale MOSFETs to this purpose. Indium atoms provide a super-steep retrograde well (SSRW) doping profile in the channel. The SSRW distribution of impurities implies a sufficiently large ratio of the maximum concentration to the surface one [1,2].

In several articles are presented the experimental results of impurities distribution of boron and indium in the channel of MOSFETs. These results were obtained by secondary ion mass spectroscopy. These results provide a comprehensive properties description of already developed devices but do not contribute to the appropriate choice of processing modes on the stage of devices development. Thus, unfortunately, an absence of physical process models complicates an appropriate choice of processing modes for nanoscale transistors manufacturing [3].

This paper presents the simulation results of the impurities distribution of boron and indium in silicon. The results were obtained for ions with initial energy up to 10 keV. The ion implantation with such ion energies is typically used at manufacturing of nanoscale MOSFETs. The impurities distribution was conducted immediately after implantation and after subsequent annealing in inert and oxidizing ambient. At such technological processes, after ion implantation, for impurity activation and crystal lattice defect removal, the high-temperature annealing is needed [4].
2. Simulation

The one-dimensional approximation was used at the simulation. The impurities distribution was simulated by the Gaussian function. The true distribution of impurities in most cases is much more precisely described by the Pearson function. At the depths exceeding the ions mean range, the impurity concentration values, calculated by the Pearson function, practically coincide with the values, calculated by the Gaussian function. At the depths, smaller then the ions mean range, the experimental values of the impurities concentration coincide with the values, calculated by the Pearson function, and greatly exceed the values, calculated by the Gaussian function. Moreover, these differences are increased with the increasing of initial ions energy. To obtain the small doping depth, ion implantation is carried out at low initial ions energy. At that the differences between the values of impurity concentration, calculated by the Pearson function and the Gaussian function, becomes insignificant. Therefore, the use of the Gaussian function, in this case, is acceptable. This approach provides quite an accurate description of the low energy ion implantation process.

Post-implant distribution of impurities was calculated using the following expression:

\[
N(x) = \frac{Q}{\sqrt{2\pi\Delta R_p}} \cdot \exp\left[-\frac{1}{2} \left(\frac{x-R_p}{\Delta R_p}\right)^2\right],
\]

where \( x \) is the coordinate, counted from the substrate surface into depth; \( Q \) is the radiation dose, equal to the number of ions, bombarding a surface unit of the substrate during the implementation; \( R_p \) is the ion mean range in silicon; \( \Delta R_p \) is the standard deviation of ion mean range in silicon. The values of ions mean range and standard deviation were calculated according to the stopping Lindhard-Scharff-Schiott theory [5,6]. Obtained results are shown in table 1.

| Ions type | Boron | Boron | Boron | Indium | Indium | Indium |
|-----------|-------|-------|-------|--------|--------|--------|
| Ion energy, keV | 1 | 5 | 10 | 1 | 5 | 10 |
| \( R_p \), nm | 8,586 | 18,250 | 33,274 | 1,135 | 5,840 | 8,924 |
| \( \Delta R_p \), nm | 3,142 | 6,681 | 12,182 | 0,368 | 1,893 | 2,892 |

Using expression 1 and values of table 1 were obtained post-implant distributions of boron and indium ions in silicon, shown in Fig. 1. The simulation was conducted for ions with low initial energies (1, 5 and 10 keV). The radiation dose was assumed to be equal \( 3 \cdot 10^{13} \) cm\(^{-2} \). Smooth curves were obtained with interpolation by the method of the cubic spline using software Origin Pro 9.1 (Origin Lab corp.). As can be seen from Fig. 1, with the decreasing of the initial energy of ions, the concentration gradient of both impurities increases sharply. At the same modes of implementation (dose and ions energy), indium ions provide a steeper distribution of impurity, than boron ions. At that, the maximum concentration of indium ions is located closer to the substrate surface than it is typical for boron ions. However, post-implant impurities concentration on the substrate surface is too high. It does not allow providing SSRW impurities distribution, which is necessary to the formation of the channel of the nanoscale transistor with a low threshold voltage.

For the reduction of crystal lattice defects and impurity activation after ion implantation, it is necessary to carry out the high-temperature annealing of silicon substrates. During the annealing, due to the diffusion, the impurity distributes into the depth of the substrate. This leads to the reduction of impurity concentration on the substrate surface, as well as to decrease of the maximum impurity concentration. The distribution of impurities after implantation and subsequent annealing in an inert ambient at the temperature of 1000 degrees of Celsius for 10 seconds was calculated using the following expression:

\[
N(x, t) = \frac{Q}{\sqrt{2\pi(\Delta R_p^2 + 2D_t)}} \cdot \exp\left[-\frac{1}{2} \left(\frac{x-R_p}{\Delta R_p^2 + 2D_t}\right)^2\right],
\]
where $D$ is the diffusion coefficient of impurity in silicon. The values of the diffusion coefficients were calculated according to [5], and amounted for indium $5.81 \times 10^{-15} \text{ cm}^2/\text{c}$ and for boron $3.09 \times 10^{-13} \text{ cm}^2/\text{c}$. The distributions of boron and indium ions in silicon were obtained and shown in Fig. 2. As can be seen from Fig. 2, both for indium and boron the ratio of the maximum to surface concentration is decreases. For boron this ratio decreases by one order of magnitude. For indium this ratio decreases by two orders of magnitude. This indicates that the annealing in inert ambient contributes to the violation of SSRW distribution for both impurities.

![Graph showing the post-implant distribution of boron and indium ions in silicon: solid curves for indium, dashed curves for boron. Initial energy of ions: 1,4 – $E= 1 \text{ keV}$; 2,5 – $E= 5 \text{ keV}$; 3,6 – $E= 10 \text{ keV}$.](image-url)

**Figure 1.** Post-implant distribution of boron and indium ions in silicon: solid curves for indium, dashed curves for boron. Initial energy of ions: 1,4 – $E= 1 \text{ keV}$; 2,5 – $E= 5 \text{ keV}$; 3,6 – $E= 10 \text{ keV}$. 
Figure 2. Distribution of boron and indium ions in silicon after implantation and subsequent annealing in inert ambient: solid curves for indium, dashed curves for boron. Initial energy of ions: 1,4 - $E = 1$ keV; 2,5 - $E = 5$ keV; 3,6 - $E = 10$ keV.

During the annealing in oxidizing ambient except for the diffusion processes have a significant impact on the processes of impurities redistribution due to the segregation at the interface Si - SiO$_2$. The essence of the segregation process is consisting of the redistribution of impurity between Si and SiO$_2$. This process is determined by the segregation coefficient $k$, equal to the ratio of the equilibrium concentration of impurity in silicon oxide to concentration in silicon. The segregation coefficients of the impurities have been taken equal 3 for boron and 10$^3$ for indium [5,7,8]. The distribution of impurities after implantation and subsequent annealing in an oxidizing ambient at the temperature of 1000 degrees of Celsius for 60 seconds was calculated using the following expression:

$$N(x, t) = \frac{N_0\Delta R_p}{2\sqrt{\pi D t}} \left[ \exp \left[ -\frac{(x-R_p)^2}{2\Delta R_p^2 + 2D t} \right] \right] \times \left( 1 + \text{erf} \left[ \frac{R_p\sqrt{D t}}{\sqrt{\Delta R_p^2 + 2D t}} \right] + \frac{x\Delta R_p}{2\sqrt{D t(\Delta R_p^2 + 2D t)}} \right) +$$

$$\frac{1-\alpha}{1+\alpha} \exp \left[ -\frac{(x+R_p)^2}{2(\Delta R_p^2 + 2D t)} \right] \times \left( 1 + \text{erf} \left[ \frac{-R_p\sqrt{D t}}{\sqrt{\Delta R_p^2 + 2D t}} \right] - \frac{x\Delta R_p}{2\sqrt{D t(\Delta R_p^2 + 2D t)}} \right), \quad (3)$$

where $N_0 = \frac{Q}{\sqrt{2\pi\Delta R_p}}$ is the maximum concentration of impurities at ion implantation; $\alpha = k \times \frac{D_1}{D}$, where $D_1$ is the diffusion coefficient of impurity in silicon dioxide [8].

Fig. 3 presents the distributions of impurities, implanted into silicon with an initial energy of 10 keV, with subsequent annealing in an oxidizing ambient. Also, for comparison, Fig. 3 shows post-implant distributions of boron and indium ions in silicon. At the figure can be seen, that only indium ion
characterized by SSRW impurity distribution. At that, the concentration and depth of indium implantation meet the requirements for nanoscale MOSFETs.

![Graph showing impurity distribution](image)

**Figure 3.** Distribution of impurities implanted into silicon with energy 10 keV: solid curves for indium dashed curves for boron. 1,3 – post-implant distributions; 2,4 – post-anneal distributions.

### 3. Conclusion

At the simulation on the basis of calculating stopping coefficients were obtained distributions of indium and boron ions in silicon before and after annealing. It was revealed, that indium ions provide steeper impurity distribution, in comparison with boron. The post-implant ratio of the maximum to a surface concentration of an impurity for boron equal 40, and for indium equal 100. But such values of the ratio are insufficient for SSRW for MOSFETs. It was shown, that subsequent annealing in inert ambient leads to decrease of this ratio for both impurities. This annealing mode does not provide the required steepness of the retrograde distribution in the gate region of nanoscale MOSFETs for both impurities. It was also shown, that annealing for indium ions in oxidizing ambient leads to increase of this ratio by one order of magnitude. This ensures SSRW distribution of impurity. Thus, it was demonstrated, that the SSRW distribution of indium atoms is provided exactly by the annealing in an oxidizing ambient. At the same time was revealed, that the annealing of boron ions in the oxidizing ambient leads to decrease of this ratio by one order of magnitude, as well as the annealing in the inert ambient. This is because indium characterized by a much higher value of the impurity segregation coefficient. Thus, it was shown, that indium doping of the gate region contributes to suppression of the short-channel effects in nanoscale transistors, unlike boron doping. The results of this report allow to correctly approach the selection of the processing modes at nanoscale MOSFETs manufacturing.
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