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Anomalous phosphorus diffusion in Si during postimplantation annealing

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The transient behavior of P diffusion in Si implanted with As or Ge above the amorphizing threshold has been investigated. Annealing at 720 °C after Ge implantation induces extensive P segregation into the extended defect layer formed by implantation damage. This segregation is attributed to P trapping to end-of-range {311} defects and dislocation loops. For As implantation, P segregation was also observed only after 1 min annealing. However, in contrast to the Ge implantation, in the As-implanted samples, significant P depletion occurs in the As-tail region after further annealing. Nonequilibrium simulation that takes into account both Fermi-level and electric field effects shows the P depletion during transient enhanced diffusion. Furthermore, simulation results based on the coexistence of neutral and positively charged phosphorus-interstitial pairs agree well with the obtained experimental results. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379359]

Dopant profile engineering for source/drain (S/D) and extension regions is an important factor in controlling the threshold voltage of metal–oxide–semiconductor field-effect transistors (MOSFETs). In fabricating *n*-MOSFETs, arsenic ions are implanted for junction formations. The damage generated by the implantation causes As transient enhanced diffusion (TED) as well as channel boron redistribution. The B segregation in the As-tail region causes a B depletion in the space-charge layer, which leads to threshold voltage roll-off.[1] To date, B segregation has been explained primarily to be a result of B trapping to/around end-of-range (EOR) dislocation loops[1,2] and B drift migration due to the internal electric field.[3,4]

Recently, phosphorus has been implanted into the S/D regions with As in an effort to decrease the junction leakage current and the reverse short-channel effect of the 0.13 μm *n*-MOSFET.[5] The literature contains several reports on codiffusion of As and P, many of which account for the effect of implantation damage or Fermi level,[6,7] but not for the electric field because of nonuniformly doped P. In the present study, the interaction between P and both extended defects and electric field was examined by comparing the diffusion profiles of P following Ge and As implantation. Experimental and simulation results strongly suggest that the earlier-described electric field has an effect on P diffusion around the As-tail region.

The starting materials were uniformly P-doped (100) Czochralski-Si wafers having a thermally grown 12 nm screen oxide. Either Ge or As was implanted into the wafers at 30 keV to a dose of $5\times10^{14}\,\mathrm{cm}^{-2}$. Each implantation at this dose is sufficiently high so as to form an amorphous layer from the surface. Ge was chosen for implantation because this element is electrically neutral impurity in SI and has a mass that is closest to As among all of the elements. The background P-doping level was approximately $2.5\times10^{17}\,\mathrm{cm}^{-3}$. Postimplantation annealings were performed in a prewarmed furnace at 720 °C for 1–300 min in N_2 ambient. After removal of the oxide layers, the impurity profiles were measured using a Physical Electronics 6600 quadrupole secondary ion mass spectrometry (SIMS) with a cesium beam.

Figure 1 shows SIMS profiles of P in the Ge-implanted samples before and after annealing for 1, 30, and 300 min at 720 °C, together with Ge profiles. Phosphorus atoms begin to segregate in the EOR region after only 1 min annealing. This is attributed to EOR {311} defects capturing P atoms because the growth of EOR dislocation loops is slower than that of the {311} defects.[8] After annealing for 30 min, the P segregation peak becomes sharp, resulting in the depletion of P on both sides exterior to the defect layer. The P profile shows a clear peak after further annealing, for 300 min, whereas the Ge profile shows no TED. The persistence of the P segregation suggests that the EOR dislocation loops drive P to segregate into the dislocation layer.[9]

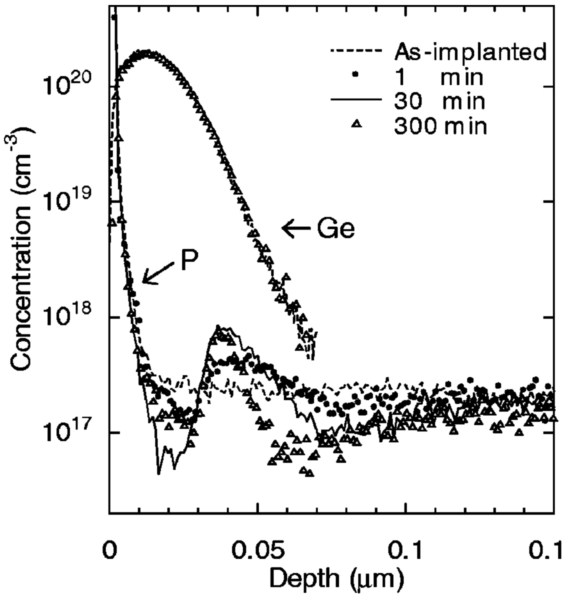

FIG. 1. SIMS profiles of P from Ge-implanted (30 keV, $5\times10^{14}\,\mathrm{cm}^{-2}$) Si before and after annealing for 1, 30, and 300 min at 720 °C, together with Ge profiles of as-implanted and annealed for 300 min.

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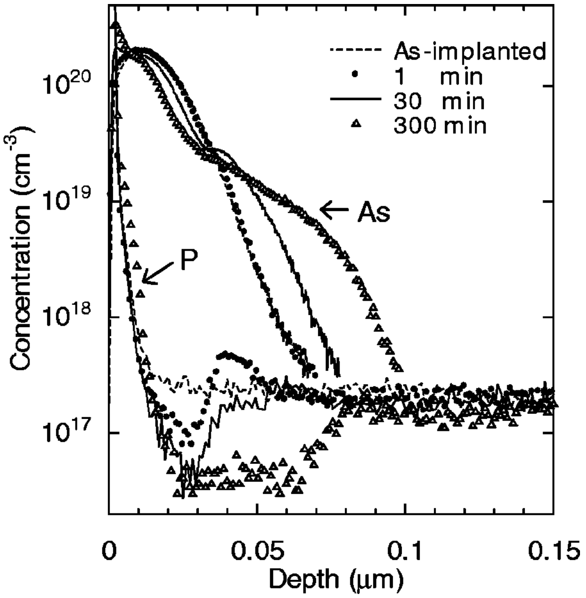

FIG. 2. SIMS profiles of P and As from As-implanted ($30\,\mathrm{keV}, 5\times10^{14}\,\mathrm{cm}^{-2}$) Si before and after annealing for 1, 30, and 300 min at 720 °C.

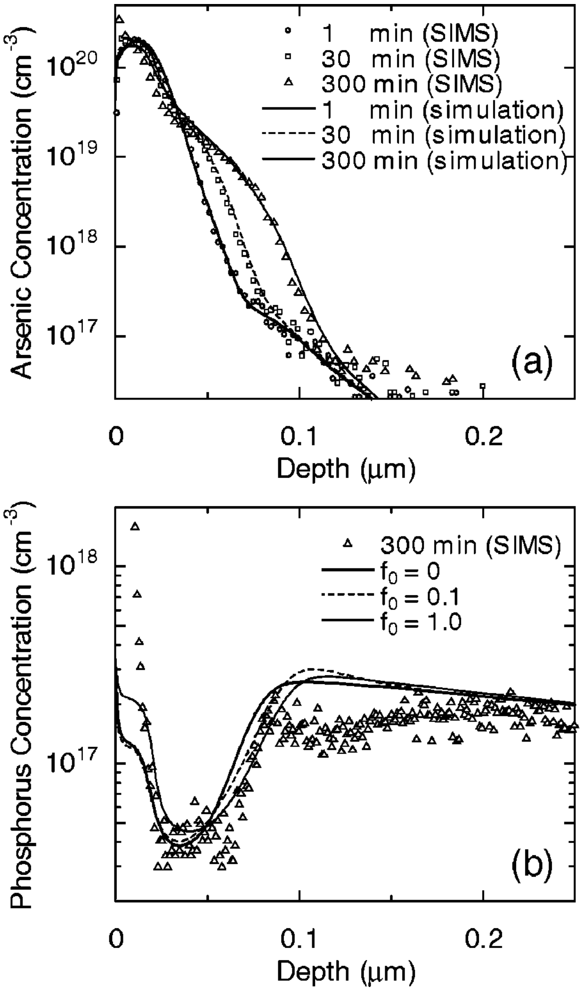

FIG. 3. Comparison of SIMS profiles and simulation results for samples implanted with As and annealed at 720 °C. (a) As profiles from samples annealed for 1, 30, and 300 min, (b) P profiles from samples after annealing for 300 min.

Figure 2 shows SIMS profiles of P and As in the As-implanted samples before and after annealing for 1, 30, and 300 min at 720 °C. After annealing for 1 min, a phosphorus segregation to EOR defects occurs in the same way as in the case of Ge-implantation (Fig. 1). During the 30 min annealing, the As tail moves to the bulk to a large degree due to TED. However, unlike the Ge-implanted case (Fig. 1), the segregation peak of P at 40 nm from the surface disappears. Moreover, the longer 300 min annealing depletes P considerably in the As-tail region as shown in Fig. 2, although a lot of EOR dislocation loops still remain in this annealing stage (Fig. 1). The P redistribution is quite different from the B redistribution,[1,3] in which B segregates into the As-tail region from the bulk.

The anomalous P behavior during TED can be attributed to both the effect of the Fermi level and that of the electric field originated from As activation. Since P diffusion is primarily mediated by silicon self-interstitial (I),[10] neutral and positively charged phosphorus-interstitial pairs, PI^+ and PI^0, have been considered in the following simulation. Under the assumption of local equilibrium on the pairing reactions, the fluxes of each pair in electric field $\mathbf{E}$ are given by

$$J_{PI^+} = -\frac{D_P^0}{C_{I^0}^{\mathrm{eq}}}\left(\frac{\partial C_{P^+}}{\partial x}C_{I^0} + C_{P^+}\frac{\partial C_{I^0}}{\partial x} - \frac{q}{k_BT}C_{P^+}C_{I^0}\mathbf{E}\right), \tag{1}$$

$$J_{PI^0} = -\frac{D_P^-}{C_{I^0}^{\mathrm{eq}}}\left(\frac{n}{n_i}\right) \times\left(\frac{\partial C_{P^+}}{\partial x}C_{I^0} + C_{P^+}\frac{\partial C_{I^0}}{\partial x} - \frac{q}{k_BT}C_{P^+}C_{I^0}\mathbf{E}\right), \tag{2}$$

where D_P^0 and D_P^- are the P diffusivities attributed paring with neutral and negatively charged interstitials, C_{P^+} and C_{I^0} are the concentrations of ionized P and neutral self-interstitial, the superscript eq denotes the equilibrium condition, and n and n_i are the concentrations of electron and intrinsic carrier. These equations indicate that the electric field pushes each pair away from the As-tail region. In particular, Eq. (2) includes a flux of PI^0 from the peak of the As profile to the surface and to the bulk due to the high concentration local electrons. Therefore, after the longer annealing, such effects as electric field and Fermi level would overwhelm the driving force of P segregation to the EOR dislocation layer, as observed in the Ge-implanted sample.

We performed numerical simulation in order to verify the earlier-described P depletion mechanism by dynamically solving the five-stream model, taking both the Fermi-level effect and the electric field effect into account. Since the growth and dissolution of extended defects strongly affect TED, the models of {311} defects and dislocation loops are also included in the simulation. In order to simplify the analysis of the results, the P segregation to EOR defects is ignored in the calculation. In the simulation, we kept the sum of D_P^0 and D_P^- to be equal to the intrinsic P diffusivity,[11] D_P^i, according to the following relationship:

$$D_P = D_P^0 + D_P^-(n/n_i) = f_0 D_P^i + (1-f_0)D_P^i(n/n_i), \tag{3}$$

where f_0 is the fractional component of the P diffusivity via neutral interstitial, or the P diffusivity via PI^+. Changing the f_0 value enables us to estimate the discrete contributions of each pair to the P depletion. Figures 3(a) and 3(b) compare the ALAMODE[12] simulation to experimental results of the As and P, respectively, for the samples implanted with As and annealed at 720 °C. In Fig. 3(a), the As-tail movements of SIMS profiles were well reproduced in all annealing stages. Figure 3(b) indicates that relatively close agreement with the experimental result are obtained by changing the f_0 value. However, the discrepancy between the measured profiles and the calculated profiles for the right-hand side of the P dip in the region of 0.05–0.08 μm, increases as f_0 decreases. According to Eqs. (1) and (2), the Fermi-level effect acts on P diffusion near the peak of the As profile, whereas the electric field effect acts in the As-tail region. This discrepancy is due to the difference in the regions over which each effect acts. The simulation results reveal that both PI^0 and PI^+ should exist in Si because the respective diffusions are partly controlled by the electric field. In addition, Fig. 3(b) indicates remarkable underestimation of the P depletion around 0.1 μm, regardless of the f_0 value. This is attributed to the lack of modeling for the P segregation into EOR dislocation loops, as observed in the Ge-implanted sample after annealing for 300 min in Fig. 1, because the segregation causes the P depletion in a deeper region than the EOR defect layer.

In conclusion, we demonstrated a significant P depletion in the As-implanted region during postimplantation annealing, which contrasts the P segregation into the EOR defect layer for Ge implantation. Simulation shows that both Fermi-level and electric field effects originated from As activation cause P depletion during TED.

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