Extended Abstracts of the 1997 International Conference on Solid State Devices and Materials, Hamamatsu, 1997, pp. 508-509 

# Simulation of 2-Dimensional Hole Gas for PMOS Devices with Phosphorus Pile-Up

Hiroshi Fujioka, Kanta Ono, Yoshiyuki Sato[1], Chenming Hu[2], and Masaharu Oshima
Department of Applied Chemistry, University of Tokyo, 7-3-1Hongo, Bunkyo-ku, Tokyo 113, Japan
Phone/Fax: +81-3-5802-8753/+81-3-5802-8629, Email: fujioka@sr.t.u-tokyp.ac.jp
[1]NTT Laboratories, Musashino-shi, Tokyo 180, Japan
[2]University of California at Berkeley, Berkeley, CA94720, USA

## 1.Introduction

It is widely known that a considerable portion of phosphorus atoms introduced by ion implantation into Si substrates segregates at the $SiO_2$/Si interface during oxidation or annealing, which is removed by a HF treatment.[1] Recently, we have shown using synchrotron radiation photoelectron spectroscopy (SRPES) and resonant Auger electron spectroscopy that the segregated phosphorus atoms exist in the silicon side of the interface. [2] Judging from the mean free path of photoelectrons in our experimental setup, the phosphorus atoms exist within a 1nm distance from the $SiO_2$/Si interface. This phosphorus pile-up phenomenon is especially important for pMOS transistors since they utilize phosphorus to control the threshold voltage. In this presentation, we will explain the effect of the phosphorus pile-up at the $SiO_2$/Si interface on pMOS devices studied with a 2-dimensional hole gas simulator.

There are two possible sites in the silicon side of the interface for the segregated phosphorus atoms, which are the interstitial sites and the substitutional sites. The phosphorus atoms at the interstitial sites should cause degradation in mobility because these atoms act as scattering centers. On the other hand, the phosphorus atoms at the substitutional sites could cause not only degradation in mobility but also Vth shift, which is very severe for the operation of MOS ICs. At the present stage, we believe that the majority of the segregated atoms are at the interstitial sites based on our experimental results with SRPES. However, it is quite natural to believe that a small portion of the segregated atoms exists at the substitutional sites, too. It is also known from the classical MOS theory that Vth is extremely sensitive to the small amount of fixed charge at the interface. The purpose of this study is to investigate the effect of the active phosphorus atoms at the $SiO_2$/Si interface on the pMOS devices using the hole gas simulator.

## 2.Simulation

We have obtained self-consistent solutions of the Shrödinger equation and the Poisson equation based on the effective mass approximation with the heavy hole band, the light hole band, and the split-off band taken into account. [3],[4] First, the Shrödinger equation is solved with a presumed electrostatic potential. In this calculation, the carrier wave functions were assumed to vanish both at the interface and at a crystal plane deep inside the substrate. After solving it, the distribution of the hole gas are calculated using the Fermi-Dirac statistics. Then, the new electrostatic potential is obtained by solving the Poisson equation. Finally, the new potential is substituted into the Shrödinger equation and the above procedure is iterated until the convergence conditions are reached.

## 3.Results and Discussion

Figure 1 shows hole distributions as a function of the depth from the interface with and without active segregated phosphorus atoms. Here, we define the segregation concentration, $N_{seg}$, as a ratio of the number of active P atoms to the number of Si sites in mono-layer. As can be seen in this figure, the replacement of only 0.3% of Si atoms of the 1st layer by the active phosphorus atoms dramatically reduces the hole concentration due to the charges of the ionized donor. In this figure, we can also see the reduction in the average distance of holes by the introduction of active phosphorus atoms, which cause reduction in the inversion layer capacitance.

Figure 2 shows the potential distribution near the interface with and without the phosphorus segregation. One can see that the band bending is suppressed due to the existence of the ionized donor. This figure also shows how the potential distribution depends upon the exact position of the phosphorus atoms. The potential distribution is sensitive to the position of the phosphorus atoms and the phosphorus atoms at the 1st site cause the most serious effect on the potential profile.

As one can imagine from these results, the threshold voltages of PMOS transistors are reduced by the electrically active phosphorus atoms. To investigate the threshold voltage shift ($\Delta$Vth), we have calculated the Vg dependence of the total hole concentration. As can be seen in Fig. 3, the total hole concentration curve shifts toward higher Vg without modifying its shape by the introduction of the segregated atoms. Since effect of segregated atoms at the interface on mobility for holes is not well understood yet, we defined the $\Delta$Vth as a difference in Vg at the weak inversion region.

Figure 4 shows how $\Delta$Vth depends upon concentration of active phosphorus atoms at the interface and the

substrate doping concentration. As you can see, ΔVth is almost proportional to the electrically active P concentration, which is consistent with the simple classical MOS theory. Since the ΔVth for the substrate doping concentrations of $1x10^{18}$ $cm^{-3}$ shows the similar values to that of $1x10^{17}$ $cm^{-3}$, we can conclude that the ΔVth is not sensitive to the substrate doping concentration for practical conditions of scaled CMOS devices. Since the number of the segregated atoms increases with decreasing process temperatures, the reduction in the wafer-to-wafer and within-a-wafer temperature distributions of the thermal process such as RTA will be essentially important for low temperature processing of the future CMOS devices.

## 4.Conclusion

We have investigated the effect of the active phosphorus atoms segregated at the SiO2/Si interface on pMOS devices using the 2-dimensional hole gas simulator. It has turned out that electrically active P atoms cause serious changes in the potential profile, the hole distribution, and the Vth even at low segregation concentrations. The potential profile near the interface is sensitive to the exact position of the active P atoms. ΔVth is proportional to the active P concentration and is not sensitive to the substrate doping concentration. Since the number of the segregated P atoms increases with decreasing process temperatures, precise control of the segregation will be necessary for low temperature processing of the future CMOS devices.

## References


1) Y.Sato, M.Watanabe, and K.Imai, J.Electrochem.Soc., 140, 2679 (1993).
2) Y.Yoshimura, K.Ono, H.Fujioka, Y.Sato, Y.Baba, K.Yoshii, T.A. Sasaki, and M.Oshima, this conference.
3) C.Moglestue, J.Appl.Phys., 59, 3175 (1986).
4) C.-Y.Hu, S.Banerjee, K.Sadra, B.G.Streetman, and R.Sivan, IEEE Electron Device Lett., 17, 276 (1996).


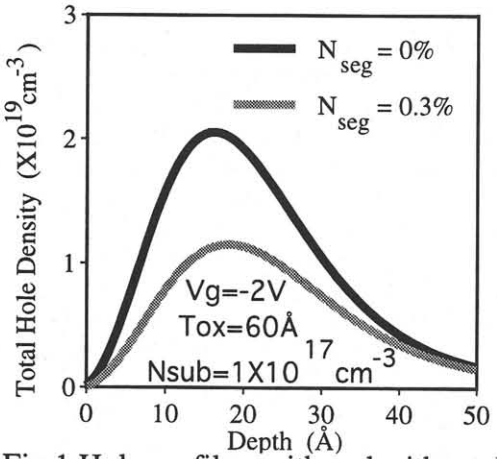


Fig.1 Hole profiles with and without P segregation.

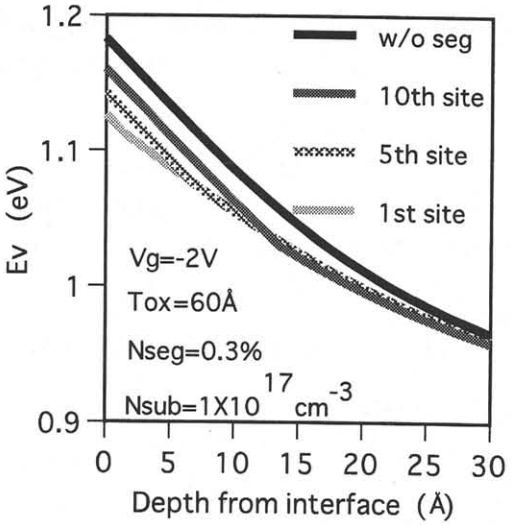


Fig.2 Potential profiles with and without P segregation.

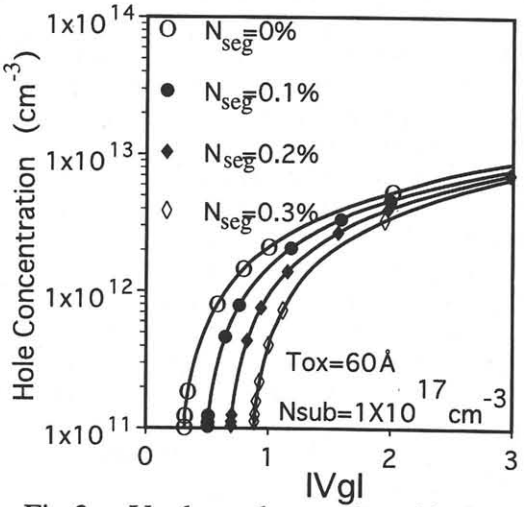


Fig.3 Vg dependence of total hole concentration.

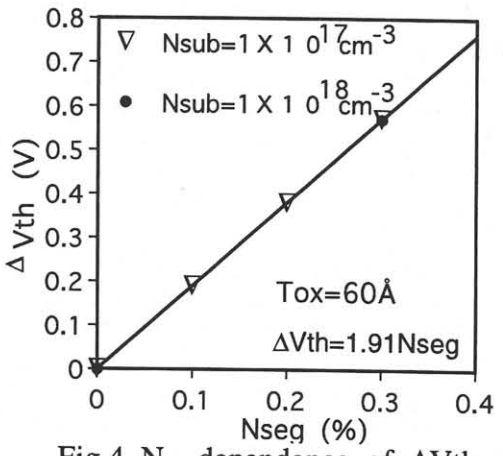


Fig.4 $N_{seg}$ dependence of ΔVth.