

Concentration Depth Profiling of Heavily Doped Boron at and near SiO₂/Si Interface by Angle-resolved Soft X-ray Photoelectron Spectroscopy

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1. Introduction

Formation of abrupt and shallow junctions in complementary metal-oxide-semiconductor (CMOS) devices has been of great importance to overcome the short-channel effect as well as to reduce the parasitic resistance. Accordingly, characterization of the surface and interface of the junctions with sub-nanometer resolution in depth is becoming an important issue. Commonly, secondary ion mass spectroscopy (SIMS) has been performed to extract the depth profiling of the dopant atoms, however, SIMS suffers from errors originated from surface transient and matrix effects [1]. Recent approaches such as x-ray photoelectron spectroscopy (XPS) [2], atom probe tomography (APT) [3], high-resolution Rutherford backscattering spectroscopy (HRBS) [4] and high-resolution elastic recoil detection (HERD) [5] have been developed to extract the very surface of the substrate. Recently, precise boron depth profiling has been performed by cyclic sub-nm etching and soft x-ray photoelectron spectroscopy, where the concentration of boron atoms at surface has been extracted using small inelastic mean free path (IMFP), λ , of 1 nm [4].

Generally, the number of photoelectrons from a surface located at z , $I(z)$, are determined by the λ , cross-section (σ), and depth (x) dependent concentration ($c(z)$) from the surface as expressed in eq. (1) and fig. 1. Here, A and θ are a constant and a take-off angle (TOA), respectively. The surface concentration, $c(z)$, can be obtained via eq. (2) as eq.(3). Under a condition that $\lambda \sin \theta$ is small, the second term in eq.(3) can be neglected, which gives $c(z)=c_0$ as eq.(4). However, when a junction with abruptness (a), defined as the distance for an order of magnitude change ($c(z)=c(0)10^{-z/a}$), is measured the second term cannot be neglected as it induces errors in estimating $c(z)$, especially when steep abrupt junctions is used, as shown in fig. 2. This paper shows an angular-resolved XPS analysis of depth profiling of boron atoms taking the second term into account.

2. Experimental details

B-doped Si(100) substrates were prepared by plasma doping (PD) with a dose of 1×10^{15} cm⁻² and spike rapid thermal annealing (RTA) at 1075 °C was conducted. Detailed process is described in ref. [6]. SIMS measurement profile revealed a steep boron profile of 3 to 4 nm/decade at the surface as shown in fig. 3, so that the second term in eq.(3) cannot be neglected. The photoelectron spectra of B

1s and Si 2p were measured at SPring-8 BL27SU with a photon energy of 500 eV and take-off-angles (TOAs) from 20 to 80° as shown in fig. 4. Here, $I(\text{Si})$ and $I(\text{B})$ represents intensities of unoxidized Si and B atoms, respectively and $I(\text{SiO})$ and $I(\text{BO})$ are those at oxidized states. The followings are the procedures and assumptions for analysis.

- Surface SiO₂ has the same concentration of thermally oxidized one and sub-oxides are treated as SiO₂ [7].
- TOAs are corrected taking the surface refraction [8].
- Si 2p_{3/2} from Si 2p spectra by decomposition [9].
- IMFPs of B 1s and Si 2p_{3/2} photoelectrons in SiO₂ are fixed to 1.00 and 1.18 nm, respectively [10, 11].
- $\sigma(\text{Si } 2p_{3/2})/\sigma(\text{B } 1s)$ is 1.36.
- Initial SiO₂ film is unchanged after annealing.
- $c(z)$ was calibrated at the values obtained at $z=5\sim 10$ nm by SIMS measurement.

3. Results and discussion

Figure 5(a) shows the TOA dependence of $I(\text{Si})/I(\text{SiO})$, where the initial SiO₂ film of 0.87 nm increased to 1.47 nm after RTA. To explain the TOA trend, the IMFP in Si substrate before and after RTA can be extracted as 0.25 and 0.43 nm, respectively. Figure 5(b) shows the TOA dependence of $I(\text{BO})/I(\text{SiO})$ before/after RTA, where the initial SiO₂ layer with an additional 0.6-nm-thick-SiO₂ layer with higher boron concentration can be recognized. Figure 6 shows the TOA dependence of $I(\text{B})/I(\text{Si})$ before/after RTA, where large drop at smaller TOA is observed, indicating a large change in the depth profile. With cyclic etching and XPS measurements, a boron depth profile, shown in fig. 7, was extracted to reproduce the TOA dependent intensity ratio, where large increase in the concentration at the surface was observed. Redistribution of boron atoms can be explained by RTA induced segregation with density of 4.78×10^{13} cm⁻² and those up taken during SiO₂ formation with that of 3.77×10^{13} cm⁻². The IMFP values of B 1s in Si substrate before and after RTA are determined to be 0.35 and 0.61 nm, respectively, indicating the change in substrate crystallinity.

4. Conclusion

Angle-resolved XPS analysis of boron doped Si substrates with steep depth profile has been performed. Segregation-induced redistribution of B atoms across the SiO₂/Si interface has been found to occur during RTA.

References

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$$I(z) = A \int_0^\infty c(z+x) \sigma \exp\left(-\frac{x}{\lambda \sin \theta}\right) dx \quad (1)$$

$$\frac{dI(z)}{dz} = A \sigma \left[-c(z) + \frac{I(z)}{\sigma \lambda \sin \theta} \right] \quad (2)$$

$$c(z) = \frac{I(z)}{A \sigma \lambda \sin \theta} - \frac{1}{A \sigma} \frac{dI(z)}{dz} \quad (3)$$

under constant concentration of $c(z)=c_0$

$$c_0 = \frac{I(z)}{A \sigma \lambda \sin \theta} \quad (4)$$

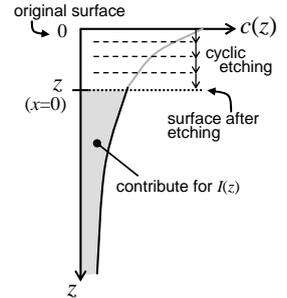


Fig. 1 An example of a dopant concentration depth profile.

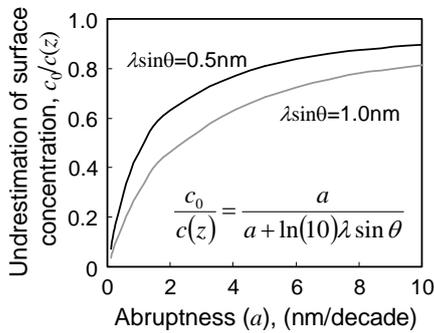


Fig. 2 Ratio of underestimation using eq.(4) and with the second term in eq.(3) on the abruptness. Error becomes large with steep concentration profile.

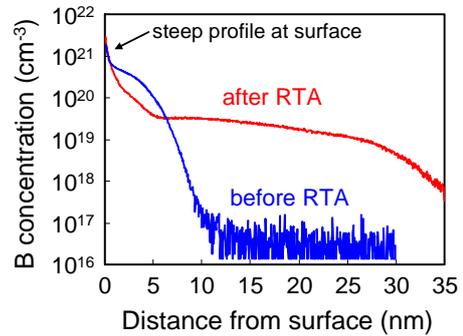


Fig. 3 SIMS profile of B atoms before and after RTA, showing a steep concentration profile at the surface.

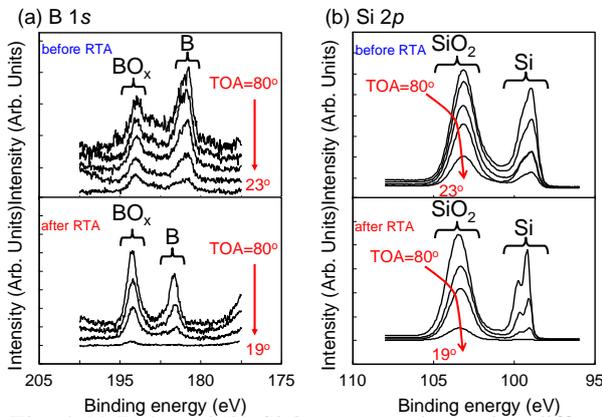


Fig. 4 (a) B 1s and (b) Si 2p spectra obtained at different TOA.

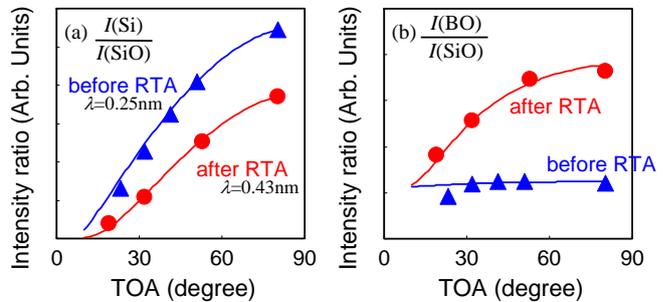


Fig. 5 Intensity ratio of (a) $I(\text{Si}/\text{SiO})$ and (b) $I(\text{BO}/\text{SiO})$ on TOA before and after RTA.

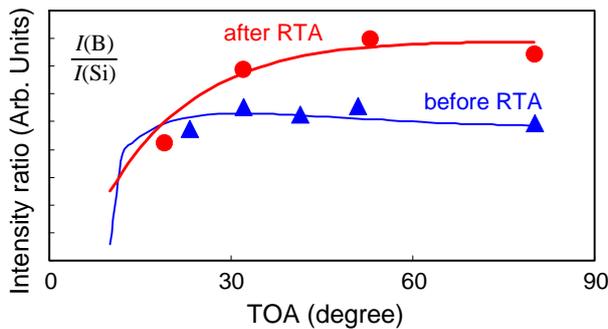


Fig. 6 Intensity ratio of $I(\text{B}/\text{Si})$ on TOA before and after RTA.

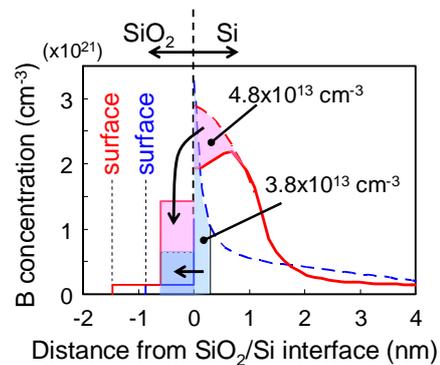


Fig. 7 Depth profile of B atoms before and after RTA, showing redistribution at the surface.