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Chemical-state-resolved in-depth profile in a SiO_2/SiN stack film studied by angle-resolved photoemission spectroscopy using synchrotron radiation

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Introduction

Si oxynitride (SiON) films are one of the most suitable gate insulators in near-future complementary metal oxide semiconductor (CMOS) devices because of applicable dielectric constant and reduction of gate-leakage currents. Precise control of nitrogen concentrations and nitrogen chemical bonding states in the films are essential to improve the characteristics of CMOS devices. Until now, extensive experimental and theoretical investigations have revealed that microscopic nitrogen bonding states including second nearest neighbor atoms affect the quality of SiON films. In order to probe the nitrogen concentrations and chemical bonding states along the depth, angle-resolved x-ray photoemission spectroscopy has been widely utilized for several SiON films. However, it is difficult in conventional x-ray photoemission spectroscopy to resolve chemical states with high accuracy because of the broadening of the spectral line width since chemical shifts derived from the second nearest neighbor effect of the nitrogen bonding states are as small as 0.7-0.8 eV.[1-3] In addition, although angular dependence of the photoemission spectra qualitatively enables to provide information on depth profiles, an elaborate numerical calculation technique to convert emission-angle profiles into depth profiles has to be established for quantitative analysis. In this study, we have performed high-resolution photoemission spectroscopy using synchrotron radiation on a SiO_2/SiN stack film to determine chemical-state-resolved depth profiles by numerical calculation based on maximum-entropy method (MEM).[4]

Experimental

A SiO_2/SiN stack film was fabricated by chemical vapor deposition methods. The SiN layer was grown using N_2-gas plasma on H-terminated Si substrates at the substrate temperature of 700 ºC. Subsequent post-oxidation was performed at 600 ºC for SiO_2 layer growth. Photoemission spectroscopy was carried out at an undulator beam line BL-2C of the Photon Factory in High-Energy Accelerator Research Organization (KEK). The total energy resolutions were 0.15 eV and 0.30 eV at $h\nu$ = 620 eV for Si 2*p* and N 1*s* core-levels, and $h\nu$ = 800 eV for Si 2*p*, N 1*s*, and O 1s core-levels, respectively. Emission angle of photoelectrons was changed from the surface normal to 60° for enhancing the surface sensitivity.

Results and Discussion

Figure 1 shows a chemical-state-resolved depth profile in the SiO_2/SiN stack film by MEM analysis. The depth profile showing a double layer structure reveals that the SiO_2 layer is distributed in the surface region and the SiN layer is partly oxidized. N1, N2, and N3 components are deconvoluted by peak-fitting procedures of N 1*s* core-level spectra in order to resolve chemical states. We assigned the N1 component as the nitrogen atoms in the $[N\text{-}Si_3]\text{-}O_xN_{9-x}$ configuration surrounded by three silicon atoms as nearest neighbor atoms and nine nitrogen or oxygen atoms as second nearest neighbor atoms. The N2 and N3 components can be assigned as $N\text{-}Si_2O$ and $N\text{-}SiO_2$ configurations, respectively, comparing the binding energies of the N2 and N3 components with the previous experimental and theoretical values.[3,5] The N2 component in the nitrogen profile exists at the SiO_2/SiON interface around 10 Å below the surface. The N3 component exists embedded in the SiO_2 matrix. Theses results suggest that N2 and N3 components are well related to the increase of oxygen concentration, which changes the chemical states of first or second nearest neighbor nitrogen atoms.

References

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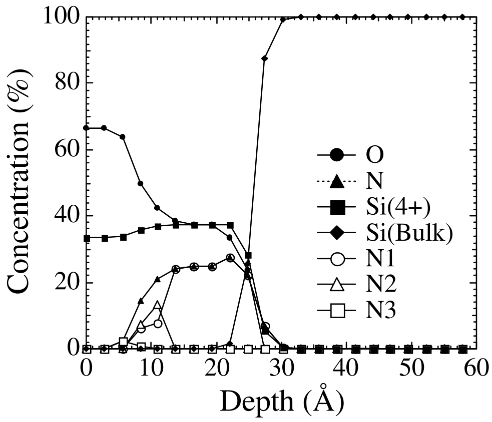

Fig. 1. Chemical-state-resolved in-depth profile of the SiO_2/SiN stack film calculated by MEM analysis.