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Microelectronic Engineering 80 (2005) 98–101
MICROELECTRONIC ENGINEERING
www.elsevier.com/locate/mee

Angle-resolved XPS study on chemical bonds in ultrathin silicon oxynitride films

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Abstract

It was found by applying maximum entropy concept to angle-resolved Si 2p and N 1s photoelectron spectra that the distribution of nitrogen atoms and their bonding configurations in oxynitride films formed by nitridation of silicon oxide in nitrogen plasma followed by annealing is quite different from those in oxynitride films formed by nitridation of silicon oxide in NO ambient. Here, the nearest neighbors of silicon and nitrogen atoms determined from the deconvolution of Si 2p and N 1s spectra were considered.

Keywords: oxynitride, depth profile, composition, chemical bonds, XPS

1. Introduction

Ultrathin silicon oxynitrides are important gate dielectrics in CMOS devices, due to their high reliability and ability to suppress boron penetration [1]. Protection against boron penetration at the SiO_2/polycrystalline silicon interface and hot carrier resistance at the SiO_2/Si interface can be attained by incorporating nitrogen atoms at these two interfaces. However, the excessive incorporation of nitrogen atoms at SiO_2/Si(100) interface increases interface roughness [2], thereby decreasing carrier mobility in the channel region. The nitridation of silicon oxide film in NO ambient has been widely used because nitrogen atoms can be incorporated mostly near the SiO_2/Si interface [3]. The nitridation of silicon oxide in nitrogen plasma (abbreviated in the following as plasma nitridation) has been used recently mainly because nitrogen atoms are considered to be selectively incorporated near the surface of the ultrathin silicon oxide film. This can be only verified non-destructively by applying maximum entropy concept to the analyses of the angle-resolved photoelectron spectra [4, 5] arising from the oxynitride films as shown in the following.

0167-9317/$ - see front matter
doi:10.1016/j.mee.2005.04.049

2. Experimental Details

Oxynitride films studied were prepared on p-type Si(100) surfaces by wet oxidation at 950°C followed by two kinds of nitridation. One was plasma nitridation followed by annealing, while another was nitridation of silicon oxide in NO ambient [5,6] at 950°C (abbreviated in the following as interface nitridation). According to the time of flight secondary ion mass spectroscopy, an oxynitride film formed by plasma nitridation followed by annealing contains maximum nitrogen concentrations of 7 at.% on the surface of the films, while an oxynitride film formed by interface nitridation contains maximum nitrogen concentration of 5 at.% at the interface. Thickness of these films as determined by XPS have equivalent silicon oxide film thickness of 1.16 and 1.10 nm, respectively. Here, values of 2.11, and 3.8 were used for the electron escape depths of the Si 2p photoelectrons in Si and that in SiO_2, respectively. The oxide film thicknesses were determined at the photoelectron take-off angle of 52°, where the elastic scattering of Si 2p photoelectrons in silicon oxide can be effectively neglected [7]. The amount and location of nitrogen atoms in oxynitride films were studied from the measurement of N 1s and Si 2p photoelectron spectra excited by Monochromatic Al Kα radiation at photoelectron take-off angle of 8, 11, 15, 20, 30, 40, 52 and 90 degrees with photoelectron acceptance angle of 3.3° at the entrance of electron energy analyser using ESCA-300 manufactured by Scienta Instruments AB [8]. Other experimental and analytical details were described elsewhere [6].

3. Results and Discussions

The nearest neighbors of a silicon atom can be determined from the analyses of Si 2p photoelectron spectra. Figure 1 shows the Si $2p_{3/2}$ photoelectron spectra measured at photoelectron take-off angle of 15° for two kinds of the oxynitride films. The Si $2p_{3/2}$ spectra chemically shifted from silicon substrate peak by 3.31 and 3.24 eV painted with grey in Fig. 1 can be correlated with a silicon atom bonded with one nitrogen atom and three oxygen atoms. It was found from the dependence of the intensity of Si $2p_{3/2}$ spectrum chemically shifted from silicon substrate peak by 3.24 eV (referred in the following as SiON spectrum) on the photoelectron take-off angle that a silicon atom bonded with one nitrogen atom and three oxygen atoms exists near the interface. The

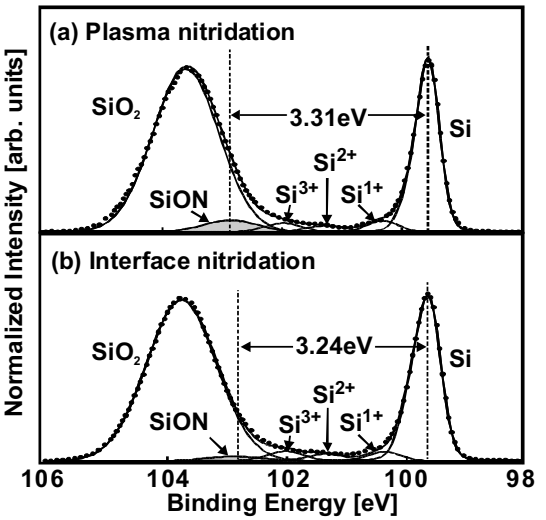

Fig. 1 Si $2p_{3/2}$ spectra measured at photoelectron take-off angle of 15° for two kinds of oxynitride films.

nearest neighbors of a nitrogen atom can be determined from the analyses of N 1s photoelectron spectra. Figure 2 shows N 1s spectra measured for two kinds of the oxynitride films at photoelectron take-off angle 90°. The deconvolution of N 1s spectra shown in Fig. 2 was performed by considering that an asymmetric part in N 1s spectrum in Fig. 2(a) appears on the low binding energy side and an

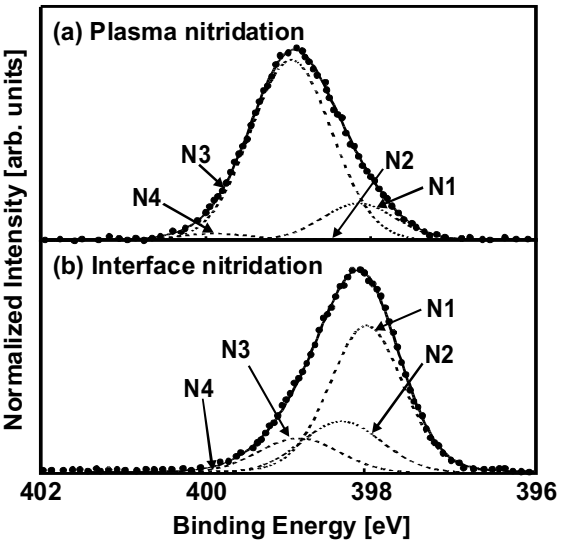

Fig. 2 N 1s spectra measured at photoelectron take-off angle of 90° for two kinds of oxynitride films.