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Study of Si(111) surfaces fluorinated by XeF_2 at room temperature using photoelectron-photoion coincidence spectroscopy

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Introduction

Fluorination of silicon surfaces by XeF_2 at room temperature is interesting as fundamental science as well as applications for dry etching processes of semiconductor devices and micromachines. Photoelectron-photoion coincidence (PEPICO) spectroscopy is a powerful means to study fluorination of silicon surfaces, because it provides F^+ yields for selected Si sites, such as SiF, SiF_2 and SiF_3, and because it probes only the top-most layer. We therefore investigated Si(111) surfaces after various XeF_2 exposures at room temperature [1] using a new PEPICO analyzer [2] at PF-8A.

Experimental

Fluorinated Si(111) surfaces (F/Si(111)) was prepared by exposing a clean Si(111)-7×7 surface to XeF_2 under 1.3×10^{-4} Pa at room temperature. Photoelectron spectra (PES) and coincidence spectra of Si 2p photoelectrons and F^+ photoions were measured with a PEPICO analyzer [2] in an ultrahigh vacuum chamber at hν = 269 eV. The incidence angle of synchrotron radiation was 84˚ from the surface normal.

Results and Discussion

For PES of F/Si(111) Si 2p components with a chemical shift of ~1, ~2, ~3 eV to the bulk Si were observed, which were assigned as SiF, SiF_2 and SiF_3 sites according to a previous PES study by Lo et al. [3]. A component with a chemical shift of ~4 eV is also observed. We call it SiFx hereafter. Figure 1 shows Si 2p photoelectron intensities of the SiF+SiF_2, SiF_3 and SiFx components divided by that of the bulk Si 2p as a function of the exposure to XeF_2. For exposures of 3200~320000 L, the SiF+SiF_2 PES component reached a constant intensity, while the SiF_3 and SiFx PES components continued to increase.

For Si 2p - F^+ PEPICO yield spectra a component with a chemical shift of ~5 eV is also observed. We call it SiFy hereafter. Figure 2 shows F^+ PEPICO yield intensities for the SiF+SiF_2, SiF_3, SiFx and SiFy components. The SiF+SiF_2 and SiF_3 PEPICO components decreased over 9600 L, while the SiFx and SiFy PEPICO components continued to increase over 9600 L. Since PEPICO probes the topmost layer, these results suggest that SiF, SiF_2 and SiF_3 change into SiFx and SiFy. So we assigned the SiFx and SiFy components to the surface $SiFSi^*F_3$ and $SiF_2Si^*F_3$ sites, respectively. We concluded that fluorination of the topmost Si layer proceeds after the initial XeF_2 exposures, while fluorination of the second Si layer starts in 6400~9600 L.

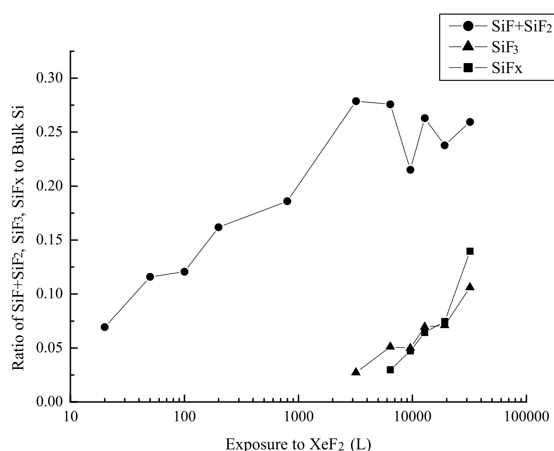

Fig. 1. Intensities of the SiF+SiF_2, SiF_3 and SiFx components of Si 2p PES as a function of exposure to XeF_2.

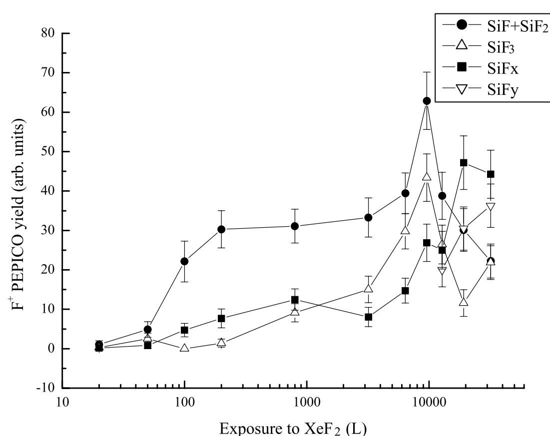

Fig. 2. Intensities of the SiF+SiF_2, SiF_3, SiFx and SiFy components of the Si 2p - F^+ PEPICO yield spectra as a function of exposure to XeF_2.

References

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