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Local Valence Electronic States of SiO_2 Ultrathin Films Grown on Si(100) Studied Using Auger Photoelectron Coincidence Spectroscopy (APECS): Observation of Upward Shift of Valence-Band Maximum as a Function of SiO_2 Thickness

Takuhiro KAKIUCHI*[1], Narihiko FUJITA[2], Masatoshi TANAKA[2],
Kazuhiko MASE[3, 4], and Shin-ichi NAGAOKA[1]
[1]Department of Chemistry, Faculty of Science, Ehime University, 2-5 Bunkyocho, Matsuyama,
Ehime 790-8577, Japan
[2]Department of Physics, Faculty of Engineering, Yokohama National University, 79-5 Tokiwadai,
Hodogaya-ku, Yokohama 240-8501, Japan
[3]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan
[4]Department of Materials Structure Science, School of High Energy Accelerator Science, the
Graduate University for Advanced Studies, 1-1 Oho, Tsukuba 305-0801, Japan

Introduction

The local valence electronic states of SiO_2 ultrathin films grown on a Si(100)-2×1 surface (SiO_2/Si(100)) have been studied extensively because (1) in-depth understanding of the electronic properties of surfaces and interfaces from an atomic point of view is of fundamental importance in science, and (2) these films play dominant roles in metal-oxide-semiconductor field-effect transistors (MOS-FETs). Therefore we investigate the local valence electronic states of the surface of the SiO_2/Si(100) ultra-thin films by using Si-$L_{23}VV$ Auger electron – Si^{4+}-2*p* photoelectron coincidence spectroscopy (Si-$L_{23}VV$-Si^{4+}-2*p* APECS, the oxidation number represents the number of oxygen bonding to Si) [1].

Results and Discussions

Figure 1 shows the Si-2*p* photoelectron spectrum of a SiO_2/Si(100) with a thickness of 2.8 Å (≈2 ML, 2.8-Å SiO_2/Si(100)). The Si-2*p* peaks are decomposed into the Si^{n+}-2*p* photoelectron components ($n = 0, 1, 2, 3, 4$). The straight dashed line at +4.1 eV represents the Si^{4+}-2*p* photoelectron kinetic energy (*PeKE*) position taken as the trigger signals for the Si-$L_{23}VV$-Si^{4+}-2*p* APECS measurements.

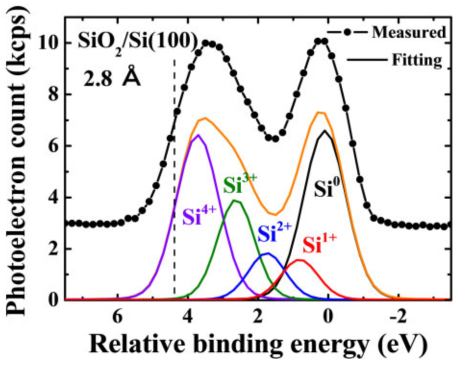

Fig. 1. Si-2*p* photoelectron spectrum of SiO_2 thermally grown on Si(100)-2×1.

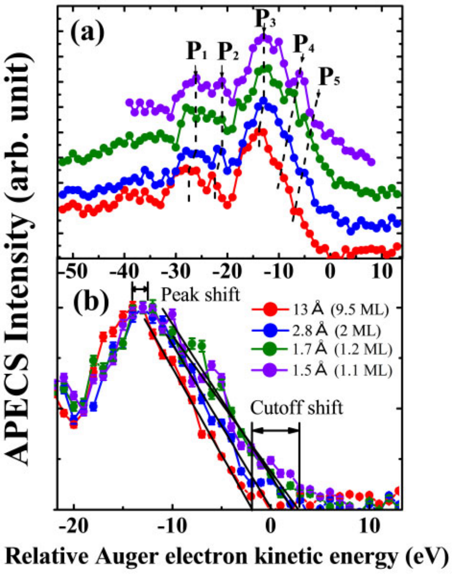

Fig. 2. Si-$L_{23}VV$-Si-2*p* APECS of SiO_2/Si(100) with the various thickness.

Figure 2 shows a series of Si-$L_{23}VV$-Si^{4+}-2*p* APECS spectra for 13-, 2.8-, 1.7-, and 1.5-Å SiO_2/Si(100). The Si^{4+}-2*p* *PeKE* positions taken as trigger signals of these APECS were set to the same value. Every wide-scan Si-$L_{23}VV$-Si^{4+}-2*p* APECS spectrum in Fig. 2(a) shows clear five peaks (P_1–P_5). In Fig. 2(b), we show the enlarged S-$L_{23}VV$-Si^{4+}-2*p* APECS spectra. The intense peaks shift by ≈1 eV to the higher-*AeKE* side, while the cut-offs shift by ≈4 eV to the higher-*AeKE* side as the SiO_2 thickness decreases. These results indicate that the binding energies of valence band maximum of 1.5- and 1.7-Å SiO_2/Si(100) are shifted upwards by ~1.6 eV (toward the Fermi level) in comparison with that of 13-Å SiO_2/Si(100) [1].

References

[1] T. Kakiuchi *et al.*, J. Phys. Soc. Jpn. in press (2011).

* kakiuchi.takuhiro.mc@ehime-u.ac.jp