

Local Valence Electronic States of SiO₂ Ultrathin Films Grown on Si(111) Studied Using Auger Photoelectron Coincidence Spectroscopy (APECS): Observation of Upward Shift of Valence-Band Maximum Depending on the Interface Structure

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Introduction

The local valence electronic states of SiO₂ ultrathin films grown on Si single crystal (SiO₂/Si) 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). Recently, We found that the valence electronic states in the vicinity of the Siⁿ⁺ site of SiO₂/Si(100) ultrathin films shift to deeper binding energies as *n* increases and that the valence-band maximum (VBM) of the SiO₂ ultrathin films shifts toward the Fermi level by about 1.6 eV as the SiO₂ thickness decreases to 1.2–1.1 ML (1.7–1.5 Å) [1]. In this study, we investigate the local valence electronic states of the surface of the SiO₂/Si(111) ultra-thin films by using Si-L₂₃VV Auger electron – Si⁴⁺-2*p* photoelectron coincidence spectroscopy (Si-L₂₃VV-Si⁴⁺-2*p* APECS, the oxidation number represents the number of oxygen bonding to Si) [2].

Results and Discussions

Figure 1 shows the Si-2*p* photoelectron spectrum of a SiO₂/Si(111) with a thickness of 3.4 Å (≈2.2 ML, 3.4-Å SiO₂/Si(111)). The Si-2*p* peaks are decomposed into the Siⁿ⁺-2*p* photoelectron components (*n* = 0, 1, 2, 3, 4). The

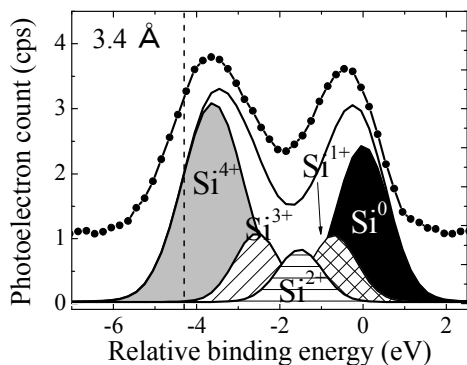


Fig. 1. Si-2*p* photoelectron spectrum of SiO₂ thermally grown on Si(111)-7×7 surface.

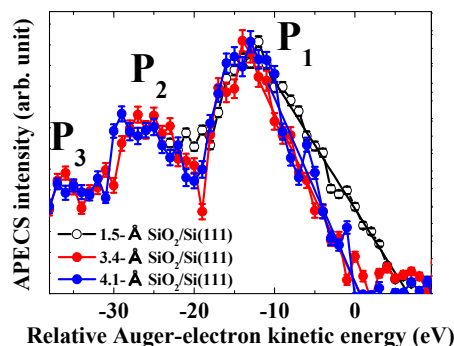


Fig. 2. Si-L₂₃VV-Si-2*p* APECS of SiO₂/Si(111) with the various thickness.

straight dashed line at +4.2 eV represents the Si⁴⁺-2*p* photoelectron kinetic energy (*PeKE*) position taken as the trigger signals for APECS measurements.

Figure 2 shows a series of Si-L₂₃VV-Si⁴⁺-2*p* APECS spectra for 4.1-, 3.4-, and 1.5-Å SiO₂/Si(111). The Si⁴⁺-2*p* *PeKE* positions taken as trigger signals of these APECS were set to the same value. Every Si-L₂₃VV-Si⁴⁺-2*p* APECS spectrum shows clear three peaks (P₁–P₃). The P₁ peaks shift by ≈1 eV to the higher-*AeKE* side, while the cut-offs shift by ≈6 eV to the higher-*AeKE* side as the SiO₂ thickness decreases. These results indicate that the binding energies of valence band maximum of 1.5-Å SiO₂/Si(111) are shifted upwards by ~2.7 eV (toward the Fermi level) in comparison with that of 4.1-Å SiO₂/Si(100). This upward shift is much larger than that of SiO₂/Si(100)-2×1. We attribute the large shift of the VBM of SiO₂/Si(111) to the formation of SiO₂ islands on the 7×7 structure and to the presence of Si¹⁺ atoms adjacent to the SiO₂ sites [2].

References

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