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Direct observation of the electronic structure at oxide/semiconductor interface by soft X-ray emission spectroscopy

Y. Yamashita* [1](13498), S. Yamamoto[1] (9972), K. Mukai[1] (13500), J. Yoshinobu[1] (13521), Y. Harada[2] (4939), Y. Takata[2] (1866), and S. Shin[1,2] (1732)

[1] ISSP, Univ. of Tokyo, [2] Riken/Spring8

The control of SiO_2/Si interfaces has been a topic of great interest because the electronic states at the interface seriously affect the performance of metal/oxide/Si (MOS) devices. Industrial gate oxide layer is currently ~ 2 nm thick and if present miniaturization trends of MOS devices continue, the gate oxide thickness will be nearing scales comparable to atomic bond lengths. Therefore, the control of the SiO_2/Si interface becomes a significant role in fabricating MOS devices. Despite its fundamental and technological importance, the electronic structure at the interface has not been reported yet. Here, we therefore report first direct observation of occupied electronic states at SiO_2/Si interface using soft X-ray emission spectroscopy and the interfacial electronic states being strikingly different from that of SiO_2 (see Fig. 1). Furthermore, on the comparison of the experimental results with theoretical calculations, it is found that anomalous atomic structures are formed at the interface and strain in the interfacial region, produced by lattice mismatch between Si and SiO_2, should be released by formation of these structures.

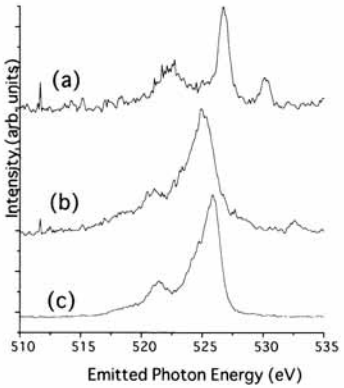

Fig. 1. O2p_O1s emission spectra of SiO_2/Si(111): (a) an O atom bonding with Si^{1+} at the interface (incident photon energy, hv, of 530 eV . (b) an O atom bonding with Si^{3+} at the interface (hv=533eV). (c) an O atom of SiO_2 (hv=537.5eV).

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The investigation of multi-electron excited states by the measurement of high resolution spectra using the coincidence with threshold electrons

T. Gejo* (8281) , M. Machida(5913), M. Nagoshi(7082)
E. Shigemasa[1] (8264), E. Nakamura[1] (8858), N. Kosugi[1] (8842), S. Masuda[1] (8843)
Himeji institute of technology, Kouto 3-2-1, Kamigori, Hyogo 678-1297, Japan
[1] *Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan*

Zero-kinetic-energy (ZEKE) electrons are emitted when the photon energy is scanned across ionization thresholds, and thus the spectroscopy based on detecting ZEKE electrons is often referred to as threshold photoelectron spectroscopy in the outer-shell ionization regions. Additional channels for producing ZEKE electrons are opened in the inner-shell excitation regions, which are mainly due to multi-electron processes such as double ionization, multiple excitations, shake-up (-off) transitions.

Recently we have developed a new technique, so-called "symmetry-resolved ZEKE spectroscopy (SR-ZEKES)", in which the combination of ARPIS (angle-resolved photoion spectroscopy) with ZEKES were used. In the beamtime of 2002B, we have successfully resolved Σ- and Π-symmetries of some spectral features related to the multiply excited states and shake-up transitions in the K-shell ionization continua of CO.

In the present experiments, we have tried to adopt the same system and compare with the photoelectron spectra of CO.

The experiments were performed at BL27SU. The threshold electron spectra was measured by penetration field type ZEKE apparatus. The photoelectron spectra was measured by a high resolution photoelectron spectra analyzer (SES-2002, SCIENTA), which is installed at c branch of BL27SU.

Fig. 1 shows the ZEKE and photoelectron spectra of CO in the K-shell region. The photoelectron spectrum was measured at a photon energy of 400eV. In these spectra, the vibrational structure has been clearly observed mainly owing to the high resolution of monochromator of BL27SU. Two spectra clearly shows the different vibrational distribution. This result indicates the different dynamical process on the different excitation energy. Based on vibrational assignment we will investigate what dynamics dominate in these excited states.

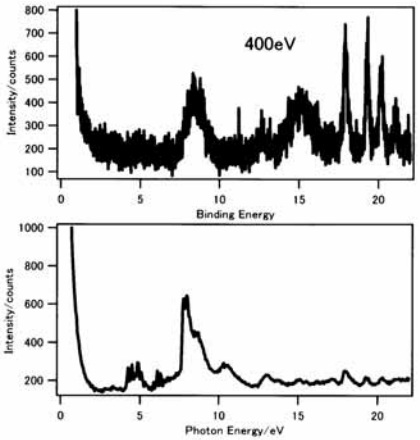

Figure 1. Photoelectron and ZEKE spectra of CO.