Surface-Site-Selective Study of Valence Electronic Structures of Clean Si(100)-2×1 Using Si-$L_{23}VV$-Si-2p Auger Electron Photoelectron Coincidence Spectroscopy

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Core-valence-valence Auger electron – photoelectron coincidence spectroscopy (*CVV*-APECS) enable us to study the local valence electronic structures at specific site of surfaces when the energy resolution of the analyzer for photoelectrons is better than the surface core-level shift. In this study, we estimated the chemical shift of highest local density of states (DOS) of Si(100)-2×1 clean surface by measuring Si-$L_{23}VV$-Si-2p Auger electron photoelectron coincidence spectrum (Si-$L_{23}VV$-Si-2p APECS) [1].

Figure 1 shows a Si-2p photoelectron spectrum of a Si(100)-2×1 clean surface at room temperature. This spectrum was decomposed into four surface components and one bulk component by a curve fitting using Voigt functions. The peak assignments are also shown in Fig. 1. The dashed lines (A)-(B) indicate the Si-2p photoelectron kinetic energy of trigger signals for the Si-$L_{23}VV$-Si-2p APECS. Figures 2 (a)-(c) shows enlarged Si-$L_{23}VV$-Si-2p APECS of clean Si(100)-2×1 measured in coincidence with Si-2p photoelectrons at the relative *BE* of (a) +0.25, (b) -0.45, and (c) +0.55 eV corresponding to the Si-2$p_{3/2}$ photoelectron peak of the Si 2nd-layer, Si-2$p_{3/2}$ photoelectron peak of the Si up-atoms, and the Si-2$p_{3/2,\ 1/2}$ photoelectron peaks of the Si 2nd layer, respectively. The black solid line is non-coincidence Si $L_{23}VV$ Auger electron spectra. The main peak of Si-$L_{23}VV$-Si-2p APECS of the Si up-atom clearly shifts by ~1 eV toward the high *AeKE* side than that of Si 2nd-layer, indicating that the energy level where the highest density of valence electronic states of the Si up-atoms shifts by 0.8 eV towards lower binding energy side relative to that of the Si 2nd-layer [1]. These results are direct evidence of the transfer of negative charge from the Si 2nd-layer to Si up-atoms.

Reference:

[1] T. Kakiuchi, S. Hashimoto, N. Fujita, M. Tanaka, K. Mase, and S. Nagaoka**,** J. Phys. Soc. Jpn.79, 064714 (2010).

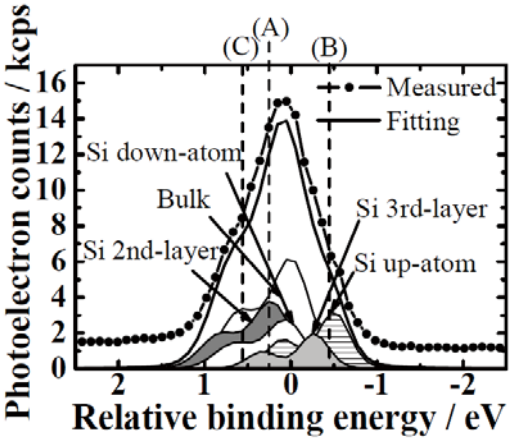

Fig. 1 Si-2p photoelectron spectrum of Si(100)-2×1 [1].

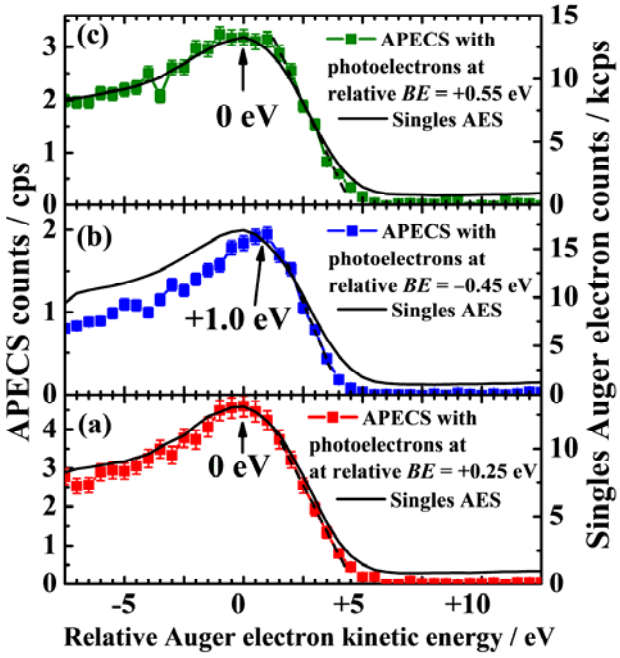

Fig. 2 Si-$L_{23}VV$-Si-2p APECS of Si(100)-2×1 [1].