Surface-Site-Selective Study of Valence Electronic Structures of Clean Si(100)-2×1 Using Si-L₂₃VV Auger Electron - Si-2p Photoelectron **Coincidence Spectroscopy**

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Introduction

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 [1,2]. In this study, we estimated the chemical shift of highest local density of states (DOS) of Si(100)-2×1 clean surface by measuring $Si-L_{23}VV$ Auger electron – Si-2p photoelectron coincidence spectrum (Si-L₂₃VV-Si-2p APECS).

Results and discussion

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- $2p_{3/2}$



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



photoelectron peak of the Si 2nd-layer, Si- $2p_{3/2}$ photoelectron peak of the Si up-atoms, and the Si- $2p_{3/2, 1/2}$ photoelectron peaks of the Si 2nd layer, respectively. The black solid line is non-coincidence Si L23VV Auger electron spectra. The main peak of Si-L₂₃VV-Si-2p APECS of the Si up-atom clearly shifts by ~1 eV toward the high AeKE side than that of Si 2nd-laver, 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 [2]. These results are direct evidence of the transfer of negative charge from the Si 2nd-layer to Si upatoms.

References

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