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Decay Processes of Si 2*s* Core Holes in Si(111)-7×7 Revealed by Si Auger Electron Si 2*s* Photoelectron Coincidence Measurements

Kazuhiko Mase,[1,2,*] Kenta Hiraga,[3] Sadanori Arae,[3] Rui Kanemura,[3] Yusaku Takano,[4] Kotaro Yanase,[4] Yosuke Ogashiwa,[4] Nariaki Shohata,[5] Noritsugu Kanayama,[6] Takuhiro Kakiuchi,[7] Shinya Ohno,[3] Daiichiro Sekiba,[5] Koji K. Okudaira,[6] Makoto Okusawa,[4] and Masatoshi Tanaka[3]

[1] Institute of Materials Structure Science, KEK, 1-1 Oho, Tsukuba 305-0801, Japan

[2] The Graduate University for Advanced Studies, 1-1 Oho, Tsukuba 305-0801, Japan

[3]Faculty of Engineering, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan

[4]Faculty of Education, Gunma University, 4-2 Aramaki, Maebashi 371-8510, Japan

[5]Institute of Applied Physics, University of Tsukuba, 1-1-1 Tennodai, Ibaraki 305-8573, Japan

[6]Faculty of Engineering, Chiba University, 1-33 Yayoi-cho, Inage-ku 263-8522, Japan

[7]Faculty of Science, Ehime University, 2-5 Bunkyo-cho, Matsuyama 790-8577, Japan

Decay processes of Si 2*s* core holes in a clean Si(111)-7×7 surface are investigated using coincidence measurements of Si Auger electrons and Si 2*s* photoelectrons at a photon energy of 180 eV. We show that Si 2*s* core holes exhibit two nonradiative decay processes: the first being a Si $L_1L_{23}V$ Coster–Kronig transition followed by delocalization of the valence hole and Si $L_{23}VV$ Auger decay, and the second being Si L_1VV Auger decay. The branching ratio of the Si $L_1L_{23}V$ Coster–Kronig transition to the Si L_1VV Auger decay is estimated to be 96.7% ± 0.4% to 3.2% ± 0.4%.

1 Introduction

The filling of an initial core hole by an electron from a higher subshell of the same shell is known as a Coster–Kronig transition, and Auger photoelectron coincidence spectroscopy (APECS), in which Auger electrons are measured in coincidence with photoelectrons with a fixed kinetic energy (KE), is an ideal tool for probing Coster–Kronig transitions because Auger electrons originating from a specific core ionization are detected [1].

However, studies of Coster–Kronig transitions have mainly been restricted to metal surfaces, even though Si surfaces are crucial for surface science applications and the semiconductor industry. Issues such as the assignments of the Si L_1VV Auger peaks, experimental determination of the branching ratio of the Si $L_1L_{23}V$ and Si L_1VV Auger decays, and competition between the delocalization of the valence hole and the Si $L_{23}V$-VVV Auger decay are, to the best of our knowledge, largely unexplored. In this paper, we report on the decay processes of Si 2*s* core holes in a clean Si(111)-7×7 surface studied using coincidence measurements of the Si Auger electron and the Si 2*s* photoelectron [2].

2 Experiment

APECS measurements were carried out in an ultrahigh vacuum chamber on the BL-11D. A clean reconstructed Si(111)-7×7 surface was prepared by direct-current heating at >1400 K for several seconds followed by slow cooling to room temperature. The sample was irradiated with *p*-polarized synchrotron radiation incident at an angle of 84° from the surface normal. The photon energy was fixed at 180 eV, and the sample temperature was maintained at room temperature.

A coincidence analyzer constructed in-house for APECS and electron–ion coincidence spectroscopy was used in the present experiments [referred to as an electron–electron–ion coincidence (EEICO) analyzer hereafter]. This EEICO analyzer, which is a modification of the previous instrument [3], consists of a coaxially symmetric mirror electron-energy analyzer (ASMA) and a double-pass cylindrical mirror electron-energy analyzer (DP-CMA). The ASMA and DP-CMA are assembled coaxially and have a common focus.

3 Results and Discussion

Figure 1(a) shows the coincidence spectrum measured by scanning the ASMA over a KE range of 20–150 eV, with the DP-CMA fixed at a KE of 76.5 eV. We refer to this spectrum as the Si-$L_{23}VV$-Si-2*p* APECS spectrum because the peak at KE = 76.5 eV corresponds to Si 2*p* photoelectrons. Distinct Auger peaks are observed in a KE region of 50–92 eV with the maximum peak located at KE = 88 eV. We assigned these peaks to Si $L_{23}VV$ Auger electrons emitted in the decay processes of Si 2*p* holes. Figure 1(b) shows the coincidence spectrum measured by scanning the ASMA over a KE range of 20–150 eV with the DP-CMA fixed at KE = 26.3 eV, which corresponds to Si 2*s* photoelectrons. We refer to this spectrum as the Si-Auger-Si-2*s* APECS spectrum. By normalizing the Si-$L_{23}VV$-Si-2*p* and Si-Auger-Si-2*s* APECS spectra by the Si 2*p* and Si 2*s* photoelectron counts, respectively, as shown in Fig. 1(c), we obtain a normalized APECS intensity that is proportional to the APECS intensity per photoemission event. The maximum peak position and shape of the normalized Si-Auger-Si-2*s* APECS spectrum in the AeKE = 50–92 eV region are almost identical to those of the normalized Si-$L_{23}VV$-Si-

2*p* APECS shown in Fig. 2(c). Therefore, we assigned these Auger peaks to Si $L_{23}VV$ Auger processes. This is direct evidence of Si $L_{23}VV$ Auger processes being induced by Si 2*s* ionization.

The peaks of Si-Auger-Si-2*s* APECS in the AeKE = 20–50 regions were assigned to Si $L_1L_{23}V$ Auger decays (Fig. 2), while the peaks of Si-Auger-Si-2*s* APECS in the AeKE = 100–150 eV regions were assigned to Si L_1VV Auger decays (Fig. 3), These results indicate that there are two nonradiative decay processes of the Si 2*s* core hole. The first is the Si $L_1L_{23}V$ Coster–Kronig transition followed by delocalization of the valence hole and Si $L_{23}VV$ Auger decay, while the second is Si L_1VV Auger decay (Fig. 4). From the integrated intensity of the normalized Si $L_{23}VV$ and Si L_1VV Auger peaks, we estimated the branching ratio of Si $L_1L_{23}VV$ to Si L_1VV Auger processes to be (96.8 ± 0.4):(3.2 ± 0.4).

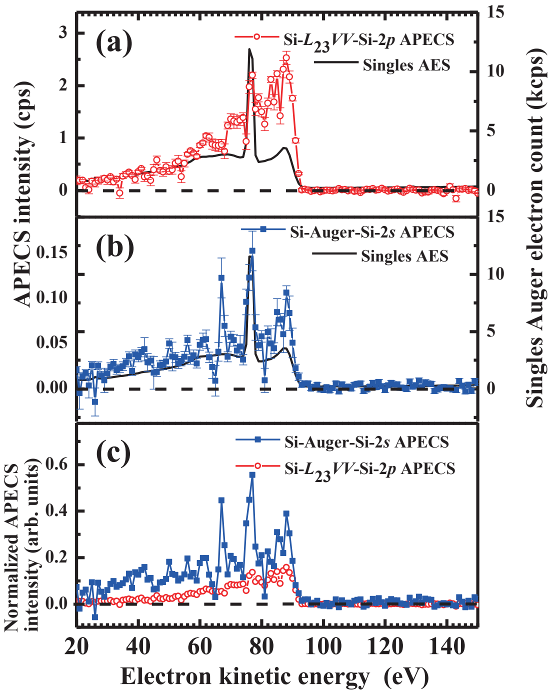

Fig. 1: (a) Si-$L_{23}VV$-Si-2*p* APECS spectrum (open circles) of Si(111)-7×7 measured in coincidence with Si 2*p* photoelectrons with a PeKE of 76.5 eV. (b) Si-Auger-Si-2*s* APECS spectrum (filled squares) of Si(111)-7×7 measured in coincidence with Si 2*s* photoelectrons with a PeKE of 26.3 eV. The photon energy was fixed at 180 eV. (c) Si-$L_{23}VV$-Si-2*p* and Si-Auger-Si-2*s* APECS spectra normalized by the Si 2*p* and Si 2*s* photoelectron counts, respectively [2].

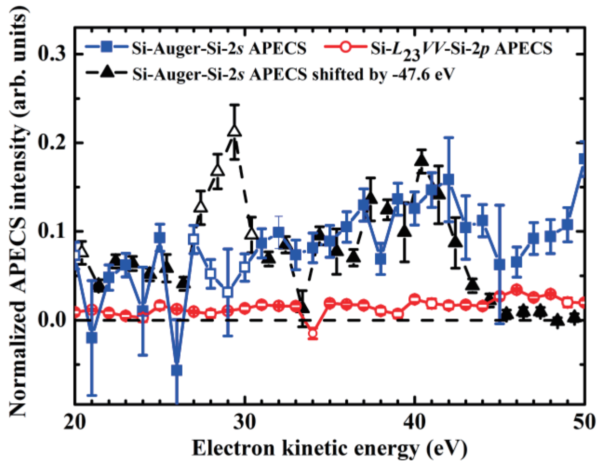

Fig. 2: Enlarged normalized Si-Auger-Si-2*s* (squares) and Si-$L_{23}VV$-Si-2*p* (open circles) APECS spectra in the electron kinetic energy region of 20–50 eV. The normalized Si-$L_{23}VV$ Auger peaks, shifted by –47.6 eV, in the Si-Auger-Si-2*s* APECS spectrum are also shown (triangles) [2].

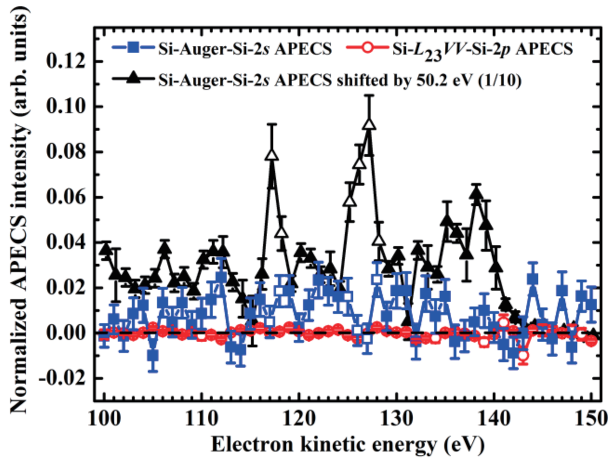

Fig. 3: Enlarged normalized Si-$L_{23}VV$-Si-2*p* (open circles) and Si-Auger-Si-2*s* (squares) APECS spectra of clean Si(111)-7×7 in the electron kinetic energy region of 100–150 eV. The normalized Si-$L_{23}VV$ Auger peaks, shifted by +50.2 eV, in the Si-Auger-Si-2*s* APECS spectra are also shown (triangles). Data shown by filled triangles and squares are used to estimate the branching ratio (see text) [2].

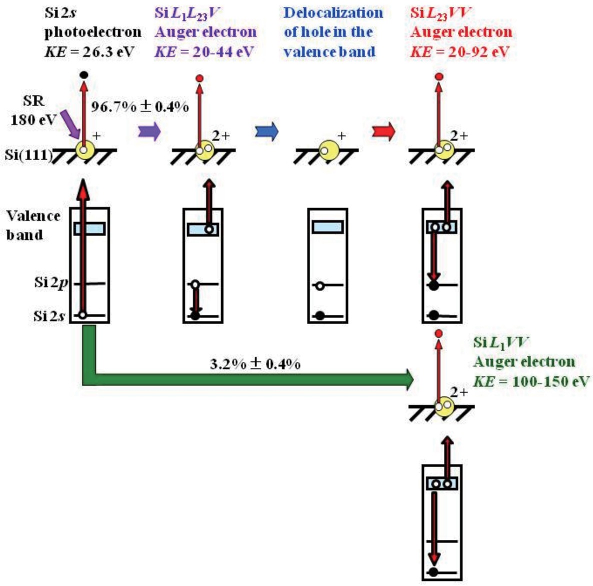

Fig. 4: Schematic drawing of the proposed decay processes of the Si 2*s* hole in Si(111)-7×7 [2].

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* mase@post.kek.jp