Surface state of Si(111)7×7 revisited: Atomic orbital characterization by Dual-beamline Photoelectron Momentum Microscopy Station at UVSOR

Fumihiko Matsui[1,2], Hiroyuki Matsuda[1], Yusuke Sato[1,2], Sakura Takeda[3], Tomohiro Matsushita[3]

[1]UVSOR Synchrotron Facility, Institute for Molecular Science, Okazaki, Aichi, Japan
[2]Sokendai, Institution, Okazaki, Aichi, Japan
[3]Nara Institute of Science and Technology, Ikoma, Nara, Japan

At room temperature, the Si(111)7×7 reconstructed surface is metallic. The Fermi level crosses the surface state S1 localized on six adatoms in the unit cell [1,2]. In recent years, remeasurements with high energy resolution have been performed, and a gap in the S1 state has been reported at low temperatures [3]. It has also been reported that the S1 state is semiconducting even at room temperature [4]. The Si(111)7×7 reconstructed surface continues to fascinate (and bewilder) researchers.

Photoelectron momentum microscope (PMM) is an analyzer that can instantaneously image the behavior of electrons of material and device surfaces. PMM combines imaging-type photoelectron spectroscopy and microscopy techniques to visualize the electronic state (band dispersion, composition, and spin polarization) in reciprocal lattice space of a selected μm-sized area. We built a PMM station [5,6] at the UVSOR Synchrotron Facility at the Institute for Molecular Science. In addition, we upgraded this advanced analyzer and experimental station to be able to use two undulator beamlines as excitation sources [7]. By branching off the existing vacuum ultraviolet (VUV) beamline BL7U, in addition to the soft X-ray (SX) beam from beamline BL6U, polarization-variable VUV light can now be used at the same time at PMM.

We developed sample holders compatible with electrical heating and revisited the band structure of the surface state using soft X-ray beamline BL6U, grazing incidence [5]. We observed the S1 band crossing the Fermi level at room temperature. We also measured the photoelectron transition matrix elements using normal incidence geometry (s-polarized light) (Vacuum Ultraviolet Beamline BL7U) [7]. Corresponding nodes were observed in the photoelectron angular distributions of the S1 (adatom) and S2 (restatom) states, which consist of p_z orbitals perpendicular to the plane, whereas no nodes were observed in the S3 (backbond) state. This corresponds to the inclusion of an in-plane p_{xy} orbital component.

Keywords: Photoelectron momentum microscope, semiconductors, surface state, atomic orbital.

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