

# Angle resolved resonant photoemission study of Si 3p band

T. Wakita<sup>a</sup>, Y. Muraoka<sup>a,b</sup>, and T. Yokoya<sup>a,b</sup>

<sup>a</sup>Research Institute for Interdisciplinary Science, Okayama University

<sup>b</sup>Research Laboratory for Surface Science, Okayama University, Okayama 700-8530, Japan

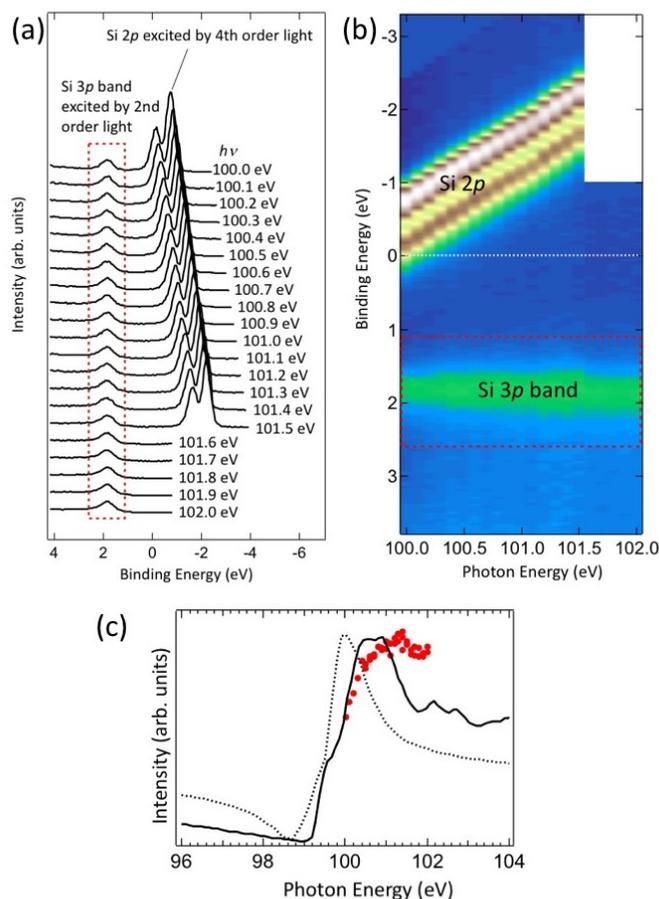
**Keywords:** Resonant photoemission, semiconductor, silicon, exciton

Resonant photoemission has been widely used to identify spectral features in valence-band photoemission spectra, for example, as *4f*- or *3d*-derived states. Such a resonance is observed when localized and highly correlated states participate to the excitation process. For band insulators with highly dispersive valence bands, some observations of resonant photoemission have also been reported in which a localized core exciton was considered to play an essential role. In 1983, Kobayashi *et al.*, for example, reported that photoemission spectra from a Si(111) cleaved surface show two types of resonant enhancement in the vicinity of *2p*-core excitation threshold, a Fano-type resonance for the *3p*-like topmost emission band and a stronger intensity enhancement in the deeper binding-energy region around 7.6 eV [1]. For the latter, they proposed that the origin is an Auger-type two-hole decay of the core exciton. A short time later, however, another explanation for these observations has been suggested, that is, both photoemission enhancements can be simulated by a non-resonant Auger signal [2]. There was a similar argument for black phosphorus based on experimental studies [3-5], and in 1986, a theoretical investigation succeeded in reproducing the above-mentioned features in valence band photoemission spectra near P *2p*-core excitation edge by using the core-exciton picture [6]. They revealed that a core exciton plays an important role both in Fano-type resonance and the enhancement of the Auger electron intensity at the core exciton threshold. In experimental spectra for black phosphorous, however, both contributions are overlapped and the experimental direct verification has been not executed still completely.

In this study, we have performed angle resolved photoemission spectroscopy (ARPES) of Si(111)1x1-H surfaces on the BL5 at HiSOR, in normal emission with various photon energies in the vicinity of Si *2p* core excitation threshold. A semispherical analyzer with an angular acceptance of  $\pm 0.5^\circ$  was used. The total energy resolutions were 0.2 – 0.3 eV in the photon energy range from 95 to 105 eV used in our measurements. The Fermi level ( $E_F$ ) position was determined by photoemission from the metallic (Mo) sample holder. The base pressure was  $5 \times 10^{-8}$  Pa. A Si(111)1x1-H surface was prepared by chemical etching in aqueous NH<sub>4</sub>F solution. All measurements were carried out at room temperature.

Figure 1 (a) shows Photon energy dependence of angle resolved photoemission spectra of a Si(111)1x1-H surface in the vicinity of Si *2p* core excitation threshold (100 – 102 eV) measured with a normal emission configuration and 2nd order synchrotron radiation. The spectra are normalized to the photon intensity. The peak at around 2 eV is the top valence band mainly originated from *3p* state (“*3p* band”). Si *2p* signals excited by 4th order lights are also included in the negative range of the binding energy of the spectra. Both signals (the *3p* band and the *2p* signal) do not overlap with each other in the photon energy range of 100 – 102 eV. Figure 1 (b) shows a 2D intensity map of the spectra. There are no Auger signals which exhibit a constant kinetic energy structure. In Figure 1 (c), we plot the integrated intensities of the *3p* band within 1.5 eV of binding energy (in the energy range shown by the red rectangles in (a) and (b)), as red circles. Although they show a clear structure, their variation behavior coincides with neither near edge structure of the Si *L*<sub>2,3</sub>-edge X-ray absorption spectrum (solid curve) nor the fit result with a Fano line-shape function (dotted curve) in ref. [1]. There are a few possible reasons for these discrepancies. (i) The photon energy dependence of the diffraction efficiency of the monochromator grating can have an effect on the photon energy dependence of the spectral intensity, since we have used the 2nd order light while the photon intensity, which we have used for the normalization of the spectral intensity, includes all orders of light. (ii) The photon energy dependence of the non-resonant photoemission cross section of Si *3p* can modify the spectral intensity owing to the empty band structure effect beyond the free electron approximation in the final state. For the former

possibility, we will experimentally investigate the photon energy dependence of the intensity of the 2nd order light in the near future. For the latter, we are now working on the theoretical calculation of the photoemission cross section of Si  $3p$  state from a Si(111) surface in a normal emission configuration. In addition, we have a plan to investigate the doping dependence of the resonant photoemission from a Si(111)1x1 surface over a wider photon energy range in order to elucidate if the carrier concentration affects the resonance energy.



**FIGURE 1.** (a) Photon energy dependence of angle resolved photoemission spectra of a Si(111)1x1-H surface in the vicinity of Si  $2p$  core excitation threshold measured with a normal emission configuration using 2nd order synchrotron radiations. The spectra are normalized to the photon intensity. (b) Intensity map of the spectra in (a). (c) The red circles show the integrated intensities of the observed Si  $3p$  band (inside the red dotted squares in (a) and (b)). The black solid curve is a Si  $L_{2,3}$ -edge x-ray absorption spectrum. The dotted curve shows the fit result with a Fano line-shape function for the photon energy dependence of the intensity of  $3p$  band observed in Ref. [1].

## REFERENCES

1. K. L. I. Kobayashi *et al.*, *Phys. Rev. Lett.* **50**, 1701 (1983).
2. R. A. Riedel *et al.*, *Phys. Rev. B* **30**, 6815 (1984).
3. M. Taniguchi *et al.*, *Solid State Commun.* **49**, 867 (1984).
4. T. Takahashi *et al.*, *Phys. Rev. B* **33**, 1485 (1986).
5. M. Taniguchi *et al.*, *Phys. Rev. B* **39**, 11160 (1989).
6. T. Nakano and A. Kotani, *J. Phys. Soc. Jpn.* **55**, 2867 (1986).