Angle-resolved photoemission study of Si electronic structure: boron concentration dependence

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Abstract

The boron concentration dependence of the Si electronic structure of Si(100)2×1 surfaces were investigated by angle-resolved photemission spectrosopy (ARPES). The ARPES spectra exhibit rigid shifts toward lower binding energy as the boron concentration increases. The band dispersion was obtained from fitting procedure, and it is found that the top of the valence band does not exceed the Fermi level even with a boron concentration 35 times larger than the critical concentration of the metal-insulator transition.

I. INTRODUCTION

Recently, superconductivity below $T_c \sim 0.35$ K was reported in Si doped with 6-8 % boron [1] and $T_c \sim 1.4$ K in SiC doped with 1-2% boron [2], following the observation of superconductivity in heavily boron-doped diamond [3, 4]. These observations have aroused much interest in changes in the electronic structures through the metal-insulator (MI) transition induced by the impurity doping for such fundamental materials. Although many experimental efforts have been dedicated to reveal the MI transition through electric conductivity measurements and other experiments [5], there are few systematic photoemission studies on the impurity concentration dependence of band insulators [6, 7]. In this study, we have performed an angle-resolved photoemission (ARPES) study of Si(100)2×1 surfaces with three different boron concentrations ($n_{\mathrm{B}} = 0.00000002$ %, 0.006 %, 0.28 %) and obtained the dispersion of Si bulk bands along the Γ-X high symmetry direction and their dependence on n_{B}.

II. EXPERIMENTAL

ARPES measurements were performed on the beam line 5 at HiSOR in Hiroshima University. A semispherical analyzer with an angular acceptance of ±1 ° was used. The total energy resolutions were 0.2-0.3 eV in the photon energy range from 100 to 200 eV used in our measurements. It should be noted that the escape depth of photoelectrons from valence bands excited with these photons are ∼ 5 Å(that is, surface sensitive). The incident angle of synchrotron radiation light and the detection angle of photoelectrons were fixed to 66 ° and 0 ° from sample surface normal, respectively. The Fermi level (E_{F}) position was determined by photoemission from the metallic (Mo) sample holder. The base pressure was 5×10^{-8} Pa. A clean Si(100)2×1 surface was prepared by heating the sample up to 1483 K for 10 s before a first measurement and repeatedly after every one-hour measurement. All measurements were carried out at room temperature.

III. RESULTS AND DISCUSSION

Fig. 1 shows the ARPES intensity maps of Si(100)2×1 surfaces measured under normal emission condition (along the Γ-X high symmetry direction), with boron concentration of

(a) n_B=0.00000002%, (b) n_B=0.02%, (c) n_B=0.28%, respectively. Their abscissa axes are calculated by using the following equation[6, 8],

$$(h/2\pi)k_\perp = [2m(h\nu - (E_B + E_0))]^{1/2} + (h/2\pi)k_{\perp\mathrm{photon}} \tag{1}$$

where h is the Planck's constant, $h\nu$ is the photon energy, $k_\perp$ and $k_{\perp\mathrm{photon}}$ are the surface normal momentum components of a photoelectron and a photon, respectively, m is the electron mass, E_B is the initial binding energy of a photoelectron, and E_0 is the zero energy for the assumed free-electron final band referred to the E_F ($E_0 = -10.3$ eV in average). It is clearly seen that a few bands are symmetrically folded back at high symmetry points in the Brillouin zone (BZ) of bulk Si (at X(003) and Γ(004)), indicating that they are bulk Si bands. Those bands shift toward lower binding energy rigidly as n_B increases.

We reproduced the spectra by fitting them with Gaussian functions to determine the peak positions precisely. Fig. 2 shows the obtained band dispersions where the areas of circles are proportional to the integrated intensities of the components. The flat features indicated by the thick arrows are the surface states and resonances of Si(100)2×1 surfaces [9]. The other flat features indicated by the thin arrows can be associated with transitions from the region of high density of states near high symmetry points in the BZ of bulk Si to the lifetime-broadened secondary-cone final states [10]. The dotted curves are theoretically calculated bands [11] whose binding energies are rigidly shifted so that the calculated features at around 3-4 eV at the X(003) correspond to the observed ones because bulk bands do not overlap with surface states there and their peak positions are determined without ambiguity. The circles, except flat features, show good agreements with the calculated bands.

Here it is noticed that the top of the valence bands for all three samples do not exceed the E_F although the boron concentration of our highest doped sample is 35 times larger than the critical concentration (n_c) of the MI transition (n_c = 0.008%, 4.06×10^{18} cm^{-3} [12]), which is strikingly different from the results for diamond [6]. We consider that there are two reasons for these observations. First, the existence of the surface states in the band gap results in a downward band bending for *p*-type semiconductor surfaces which keeps the top of the valence band away from E_F. Second, the peak top of the spectrum at the Γ point dose not correspond to the maximum edge of the valence band because of the broadening due to the lifetime and/or impurity doping. Moreover, it should be noticed that the smaller Fermi wave number at n_c for silicon than that for diamond is an additional intrinsic difficulty while searching Fermi edge of silicon near the MI transition.

Unfortunately, further analysis to access to the change in the valence band maximum and impurity band upon increasing of boron concentration is prevented by the overlaps of bulk bands with the surface states around Γ on a Si(100)2×1 surface. We have a plan to investigate the boron concentration dependence of the electronic structure with a Si(111)1×1-H surface. On this surface, the surface states are not in the band gap and far from the valence band top, which avoid the band bending and will allow us to study the change in the electronic structure around the top of the bulk valence band in detail.

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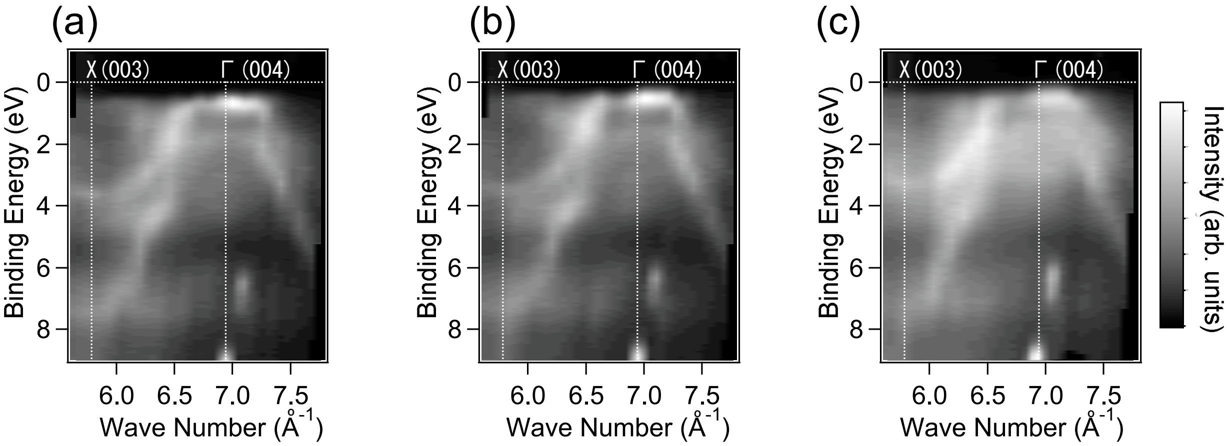

FIG. 1. ARPES intensity maps of Si(100)2×1 surfaces with boron concentration of (a) n_B=0.00000002%, (b) n_B=0.02%, (c) n_B=0.28%, respectively, measured along the Γ-X high symmetry direction.

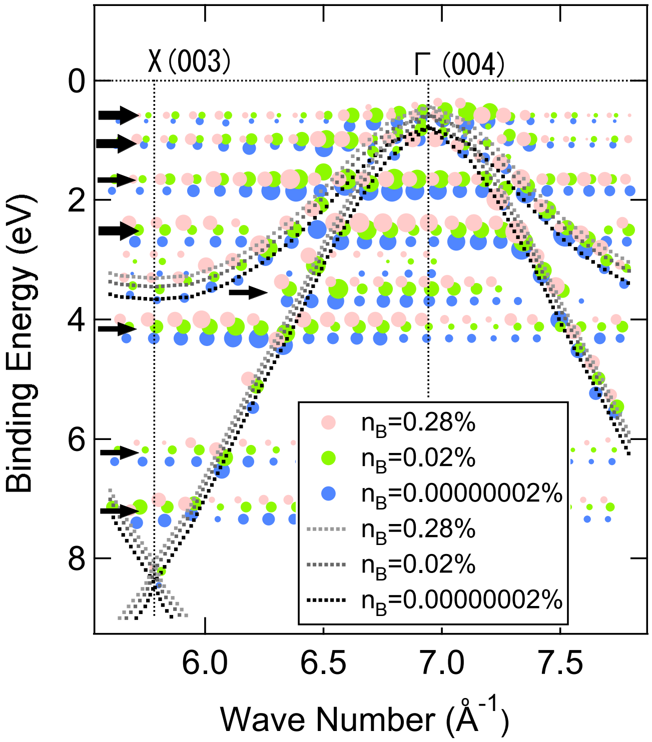

FIG. 2. Band dispersion of Si(100)2×1 surfaces obtained from fitting procedure of spectra. The areas of circles are proportional to the integrated intensities of the components. The dotted curves are the calculated bands for bulk Si [11].