Photoelectron and Synchrotron Radiation Group

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Research Activities

(I)Angle-resolved ultraviolet photoelectron spectroscopy.[1)-4)]

(1)Si(001)-(2x1)/K and Si(001)-(2x1)/Cs surface (Y. Enta, T. Kinoshita, S. Suzuki and S. Kono).

Valence-band spectra and corresponding binding energy versus wave vector diagrams for the full-coverage Si(001)-(2x1)/K and Si(001)-(2x1)/Cs surfaces show that the two surfaces are semiconducting, in contrast to a generally accepted view of the one-dimensional and metallic alkali chain of the alkali/Si(001) systems. Plausible dispersion of surface-state bands are proposed for the full-coverage Si(001)-(2x1)/K and Si(001)-(2x1)/Cs surfaces.

(2)Electronic structure of the single-domain Si(001)2x1-K surface (Y. Enta, S. Suzuki, and S. Kono)

A single-domain Si(001)2x1-K surface has been made by K deposition onto a room-temperature single-domain Si(001)2x1 substrate. The work on the single domain surface has made it possible for the first time to identify the existence of two surface-state bands and dispersions of the two bands. The resulting surface-state are in principle consistent with a recently proposed K double-layer model rather

than with the more widely believed one-dimensional alkali-metal-chain model.
(3)Addendum to empty- and filled-electronic states of the Si(111)$\sqrt{3}$x$\sqrt{3}$-Sn, $\sqrt{3}$x$\sqrt{3}$-In and 2$\sqrt{3}$x2$\sqrt{3}$-Sn surfaces (H. Ohta, T.Kinoshita, Y. Yaegashi, S. Suzuki and S. Kono).

Improvement in the KRIPS (K-resolved inverse photoemission spectroscopy) is accomplished by replacing the old incident electron gun with an improved one, which uses a BaO cathode in a Pierce-type configuration with a four-element electrostatic lens. The energy-resolution of the new KRIPS apparatus was estimated to be ~0.35 eV FWHM. Improved spectra for the $\sqrt{3}$-In and $\sqrt{3}$-Sn surfaces measured along the $\bar{\Gamma}$-$\bar{K}$-$\bar{M}$ direction of the surface Brillouin zone is consistent with a recent result of Nicholls et al.

(4)Angle-resolved ultraviolet photoelectron spectra and momentum (K)-resolved inverse photoelectron spectra of the Si(111)$\sqrt{3}$x$\sqrt{3}$-Sb surface (T. Kinoshita, Y. Enta, H. Ohta, Y. Yaegashi, S. Suzuki and S. Kono)

It has been found that at least two filled-surface-state bands exist on the $\sqrt{3}$x$\sqrt{3}$-Sb surface and that the $\sqrt{3}$x$\sqrt{3}$-Sb surface is semiconducting with a large band gap between the filled and empty-surface-state bands. Results are discussed in connection with the surface electronic structures expected for a recently proposed trimer model.

(II)Photoelectron diffraction study[5)-8)].

(1)Si(001)2x1-K surface:existence of a potassium double layer(T. Abukawa and S. Kono)

From a kinematical analysis of the diffraction patterns of K 2p core levels, it is concluded that a sawtooth-type arrangement of the potassium double array is present over the substrate. This is in disagreement with an existing assumption of the one-dimensionality of the alkali-metal-Si(001) systems.

(2)The atomic geometry of the Si(111)$\sqrt{3}$x$\sqrt{3}$-Sb(T. Abukawa, C. Y. Park and S. Kono)

The diffraction patterns of Sb 3d core levels are analyzed kinematically using a spherical and a plane-wave formalism. It has turned out that a trimer of Sb atoms is present on every $\sqrt{3}$x$\sqrt{3}$ site above the substrate. A "milk-stool" type of structure is tentatively inferred for a structural unit of the Si(111)$\sqrt{3}$x$\sqrt{3}$-Sb surface.

(3)Structural model for the negative electron affinity surface of O/Cs/Si(001)2x1 (T. Abukawa, S. Kono and T. Sakamoto)

A wide-terrace single-domain Si(001)2x1 surface has been used to prepare a single-domain Si(001)2x1-Cs surface and a negative electron affinity (NEA) surface of single-domain O/Cs/Si(001)2x1. X-ray photoelectron diffraction for the NEA surface has revealed that the Cs double-layer is preserved and adsorption of oxygen takes place in a hollow site on a level that is coplanar with the lower Cs layer.

(4)Photoelectron spectroscopy and photoelectron diffraction studies of submonolayer Metal/Si(111) interfaces (S. Kono)

A review of the recent study in our laboratory is presented. Angle-resolved ultraviolet photoelectron spectroscopy, X-ray photoelectron diffraction, maximum surface-sensitivity core level photoelectron spectroscopy are applied to the metal/Si(111) submonolayer interfaces;Si(111)/$\sqrt{3}$x$\sqrt{3}$-group III, IV, V and noble-metal surfaces.

(III)Electronic structures of high-Tc superconductors(T. Takahashi, F. Maeda and H. Matsuyama corporated with H. Katayama-Yoshida, Y. Okabe, T. Suzuki and S. Hosoya in Tohoku Univ.)[9)-22)]

(1)Ultraviolet and X-ray photoelectron study of single-crystalline $(La_{1-x}Sr_x)_2CuO_4$ with x=0.0 and 0.04[9)].

Considerable differences are found in the photoemission spectra when compared with the results for sintered samples: a single-peak structure for the O 1s level and the absence of the peak at 9eV of unknown origin reported for sintered samples, etc. Comparison is also made with band-structure calculation.

(2)Evidence from angle-resolved resonant photoemission for oxygen -2p nature of the the Fermi-liquid states in $Bi_2CaSr_2Cu_2O_8$[10)].

There has been great effort to find and characterize the electronic states at the Fermi level, because these states relate directly to the mechanism of the high-T_c superconductivity by providing Cooper pairs below T_c. Here we report the first direct evidence for the dominant oxygen -2p nature of the Fermi-liquid state in the high-T_c superconductor, obtained using the technique of angle-resolved resonant photoemission.

(3)Photoemission study of single crystal $Bi_2Sr_2CaCu_2O_8$[11)].

Two energy bands with dispersion of 0.2-0.5eV were observed in the vicinity of the Fermi level and one of them crosses the Fermi level midway between the center and boundary of the Brillouin zone, giving a clear evidence for existence of a Fermi surface. The Fermi-edge peak exhibits a pronounced enhancement at photon energy of the O 2s core threshold, meaning a dominant O 2p nature in the high-T_c superconductor.

(4)Recent research related to the mechanism of high-T_c superconductivity[12)]

i)We determined the band structure of single crystal of $Bi_2Sr_2CaCu_2O_8$ by angle-resolved resonant photoemission. Two dispersive bands with mainly oxygen 2p character were observed in the vicinity of the Fermi level and one of them crosses the Fermi level.

ii)We performed NMR study of enriched ^{17}O in the CuO_2 plane of the superconducting Y-Ba-Cu-O system and found BCS-like enhancement of ^{17}O nuclear spin-lattice relaxation rate $1/T_1$ below T_c.

iii)We observed an oxygen isotope shift in Bi-Sr-Ca-Cu-O superconductors when ^{18}O is substituted for ^{16}O. T_c is lowered by about 0.32 K for the higher-T_c phase (T_c=110 K) and by about 0.34 K for the lower-T_c phase (T_c=75 K).

(5)Experimental approach to the mechanism of high-T_c superconductivity[13].

Based upon the above experimental data related to the mechanism of super conductivity, we discuss possible electronic structure of high-T_c superconductors.

(6)Growth and characterization of $YBa_2Cu_3O_{7-\delta}$ large single crystals of high-Tc superconductors[14]

$YBa_2Cu_3O_{7-\delta}$(T=90 K) and $(La_{1-x}Sr_x)_2CuO_{4-\delta}$ (T-20 K) have been successfully grown in the cavity of the bulk materials with a CuO flux. Resistivity, Meissner effect and photoemission spectrum were measured for the single crystals. We also studied the newly discovered superconductor $BiSrCaCu_2O_x$ with T_c of 75~110 K.

(7)Oxygen isotope effect in the superconducting Bi-Sr-Ca-Cu-O system[15]

An oxygen isotope effect is observed in mixed-phase Bi-Sr-Ca-Cu-O superconduc tors when ^{18}O is substituted for ^{16}O. The superconducting transition temperature T_c, measured by electrical resistivity and magnetic susceptibility, is lowered by about 0.32 K for higher-T_c (110 K) phase and by about 0.34 K for the lower-T_c (75 K) phase. These results suggest a measurable contribution to the superconductivity from phonons.

(8)NMR and NQR studies of ^{17}O and ^{63}Cu in CuO_2 plane of high-T_c $YBa_2Cu_3O_{6.65}$ with T_c=61 K[16].

The microscopic property of each oxygen and copper site in the CuO_2 plane of $YBa_2Cu_3O_{6.65}$ with T_c=61 K has been investigated by ^{17}O NMR and ^{63}Cu NQR techniques. It has been found that the nuclear spin-lattice relaxation rate $1/T_1$ for Cu sites is depressed by three orders of magnitude as compared with that for $YBa_2Cu_3O_7$ with T_c=92 K, whereas $1/T_1$ for oxygen sites exhibits a rather small change, decreasing approximately to one-fourth (1/4).

(9)Anomalous nuclear relaxation and Knight shift behaviors of ^{205}Tl in high-T_c $Tl_2Ba_2CaCu_2O_{8+\delta}$[17].

The nuclear relaxation rate, $1/T_1$, and Knight shift have been investigated between 4.2 K and 300 K by ^{205}Tl nuclear magnetic resonance for $Tl_2Ba_2Ca_1Cu_2O_{8+\delta}$ with T_c=100 K. It has been observed that there are two Tl sites possessing a different electronic state. The distinct decrease of $1/T_1$ and knight shift for both Tl sites has been found just below an onset temperature of To=115 K rather than a zero-resistance temperature of T_c=100 K.

(IV)Electronic structures and optical properties of light rare-earth compounds using synchrotron radiation (S. Sato, H. Arai coorporated with members in other institutes).

(1)4f-derived photoemission and 4f-ligand hybridization in light rare-earth

halides[23]

We have studied the 4f-derived photoemission spectra of insulating Ce, Pr and Nd trihalides by resonant photoemission spectroscopy. A double-peak structure is observed in every f spectram as in metallic Ce, Pr, and Nd compounds and is successfully analyzed in terms of the cluster model. This confirms that the two peaks arise from hybridization between the 4f and ligand p orbitals rather than from two different screening channels of the hole.

(2)Optical properties of CeO_2 crystal in the photon energy range of 2.5-40 eV[21].

Optical reflectance spectra of CeO_2 crystal have been measured in the photon energy range from 2.5 to 40 eV. A Kramers-Kronig analysis of the reflectance data has been performed to obtain the dielectric function and related functions. The observed spectral features can be explained in terms of the charge transfer and interband transitions and the atomic-like excitation of the Ce 5p core electron.

(3)Optical constants of CVD-SiC mirrors produced by different processes from 200 to 1000 eV[24].

The optical constants of seven CVD-SiC mirrors produced by different processes have been measured in the soft X-ray region (200-1000 eV) by means by the reflectance method. In spite of the difference in the production process, no dependence of the optical constants on the samples was found. The photon-energy dependence of the optical constants for CVD-SiC is represented in terms of power formulas over a range of 300-1000 eV.

(4)Time evolutional relaxation process of 4f levels in lanthanum compounds[26].

We have made a successsful observation of a very faint X-ray lines ascribed to the 5p→3d transition in lanthanum compounds, using a quasimonochromatic undulator radiation. We have found a drastic chemical effect on the relative intensity of two components of the lines. By comparing the present X-ray emission spectra with the X-ray photoelectron spectera, a time evolutional relaxation process of 4f levels was manifested.

(5)Developing a multipurpose SR beamline highly efficient in material characterization[27].

A beamline has been developed which aims at attaining a large size white beam, as well as monochromatized beam, to have wide applications for material characterization. Problems with beryllium foil deterioration and uncomfortable levels of ozone were overcome by providing an ozone suppression section.

Master Thesis (March 1989)

Natsuo Nakamura

Study of Metal/Semiconductor Submonolayer Interfaces by Ultrahigh Vacuum Scanning Electron Microscopy.

Tadashi Abukawa

Arrangement of Alkali Metals on Semiconductor Surfaces.

Hiroshi Ohta

Inverse Photoemission Spectroscopy of High-Tc Superconductors.

Publications

1)Angle-Resolved Ultraviolet Photoelectron Spectroscopic Study of Si(001)-(2x1)/K and Si(001)-(2x1)/Cs Surfaces.
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