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▶*Instrumentation and Technique*
▶*Medical Applications*
▶*Materials Science*
▶*Surface and Interface*

Spin resolved photoemission excited by VUV-circularly polarized light of Ni(110)

Akio KIMURA[1*], Masahiro SAWADA[1], Shan QIAO[2], Ayumi HARASAWA[1], Akito KAKIZAKI[1]

[1]Tsukuba Branch of ISSP, The University of Tokyo, Tsukuba, Ibaraki 305-0801, Japan
[2]The Institute of Physical and Chemical Research (RIKEN), Saitama 351-0198, Japan

We have performed spin- and angle- resolved photoemission spectroscopy for the Ni 3d valence band using vuv-circularly polarized synchrotron radiation ($h\nu=60$-80eV) at BL-28A. Photoelectrons were collected by a hemispherical electron energy analyzer and an electron spin was analyzed by our recently developed small Mott scattering detector operated at 25kV whose efficiency is 1.9×10^{-4}. The angle of incidence of the undulator light was 75° from the surface normal. The photoelectrons emitted normal to the sample surface were collected.

The definitions of the experimental spectra are tabulated in Table I. Magnetic circular dichroism (MCD) in the spin-integrated spectra can be obtained by the formula, $I_{++} + I_{+-} - I_{-+} - I_{--}$. Furthermore, $I_{++} - I_{-+}$ ($I_{+-} - I_{--}$) produces the MCD asymmetry in majority (minority) spin channel. As shown in Fig.1 (a), both of the spin integrated spectra taken at $h\nu=80$eV show the peaks around $E_B=1$eV It is found that the binding energy (E_B) of the spectrum for the plus helicity ($I_{++} + I_{+-}$) is 0.1eV lower than that for the minus helicity ($I_{-+} + I_{--}$), which results in the dispersive asymmetry in the difference spectrum between the spin-integrated spectra [Fig.1 (b)]. One can further find that the asymmetry in the minority spin channel is remarkable compared to that in the majority spin channel as also confirmed in the MCD spectra [Fig.1 (b)]. This result indicates that the MCD appeared in the spin-integrated spectrum is mainly derived by the minority spin bands. On the other hand, the observed asymmetries are not clearly recognized in the spectra excited at $h\nu=60$eV compared to those for the spectra at $h\nu=80$eV (*not shown here*). [1] MCD asymmetry in the valence band photoemission spectra of the 3d ferromagnets has been interpreted to be derived mainly from the spin-orbit (s-o) induced initial state hybridization between the electronic band states with different spatial symmetries, which has been probed by the recent angle-resolved photoemission experiments combining with the theoretical analysis based on the relativistic band structure of 3d ferromagnets. Such an hybridization is expected to be stronger for the different spatial symmetry bands with smaller energy separation. Indeed, the energy separation between Σ_1 and Σ_3 symmetry bands is much smaller (1eV) near Γ point ($h\nu=80$eV) than that at the middle point of ΓK ($h\nu=60$eV) because the Σ_1 state shows the upward dispersion whereas the Σ_3 state shows downward dispersion along Γ-K direction. [2] Thus the s-o induced hybridization is

expected to be remarkable for these bands especially near Γ point. Furthermore, our spin-dependent MCD results possibly show that the s-o induced hybridization is larger for the minority spin states than that for the majority ones.
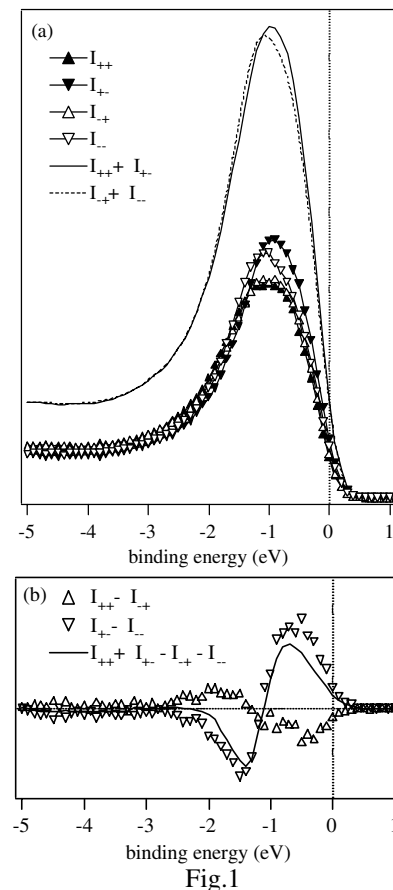

Fig.1

Table I. Definition of the experimental spectra.

I_{ab}	a: helicity of incident light	b: spin direction
I_{++}	positive ($\Delta m=+1$)	majority spin
I_{+-}	positive ($\Delta m=+1$)	minority spin
I_{-+}	negative ($\Delta m=-1$)	majority spin
I_{--}	negative ($\Delta m=-1$)	minority spin

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F. Weling and J. Callaway: Phys. Rev. B **26** (1983) 710.

* akiok@hiroshima-u.ac.jp

Spin polarized valence band photoemission from non-magnetic Cu(001)

Akio KIMURA[1*], Nozomu KAMAKURA[1], and Akito KAKIZAKI[1]

[1]Tsukuba Branch of ISSP, The University of Tokyo, Tsukuba, Ibaraki 305-0801, Japan

We have performed a spin- and angle- resolved photoemission spectroscopy (SARPES) of non-magnetic Cu(001) surface. It is known that the spin polarized electrons can be obtained from the non-magnetic surface if the circularly- or linearly- polarized light excites the photoelectron. In this report, we will show the SARPES spectra from Cu(001) surface excited by the p-polarized synchrotron radiation. The mechanism related to the yield of the spin-polarized photoelectron can be treated by the simple symmetry consideration. The finite spin polarization along the perpendicular direction to the measurement plane is expected when the photoelectron is excited by the p-polarized light [1].

The SARPES measurement was carried out at BL-19A. The angle of the incident undulator radiation is $20°$ from the surface normal. The perpendicular component to the mirror plane of the spin polarization was observed by the Mott polarimeter equipped with the hemispherical electron analyzer. The instrumental asymmetry was eliminated using the magnetized fcc cobalt thin film evaporated on Cu(001).

Fig.1 (a) shows the SARPES spectra of Cu(001) taken $h\nu$=45eV, which corresponds to Γ point in the fcc Brillouin zone. The two peak structures observed at the binding energies (E_B) of 2.6 and 3.3eV in the SARPES spectra can be assigned to the states with Δ_1 and Δ_5 spatial symmetries. It is noticed that the Δ_1 symmetry state has the negative spin polarization, whereas the Δ_5 symmetry state has the positive spin polarization. Fig.1 (b) shows the SARPES spectra taken at $h\nu$=69eV, corresponding to the middle point of the Δ line. It is found that the structure with the positive spin polarization is located at the lower E_B and the structure with the negative spin polarization is at the higher E_B and they are closer in energy compared to those of the spectra taken at $h\nu$=45eV. The relativistic band structure calculation shows that the Δ_5 and Δ_1 symmetry states are closer at the middle point of the Δ line and are strongly hybridized in the presence of the spin-orbit interaction [2]. The calculation also shows that the dominant characters of the states at the lower and higher binding energies are Δ_5 and Δ_1 at this middle k point, respectively, which are opposite to the case at the Γ point [2]. This is consistent with the change of the spin polarization in the SARPES measurements taken at the different excitation energies.

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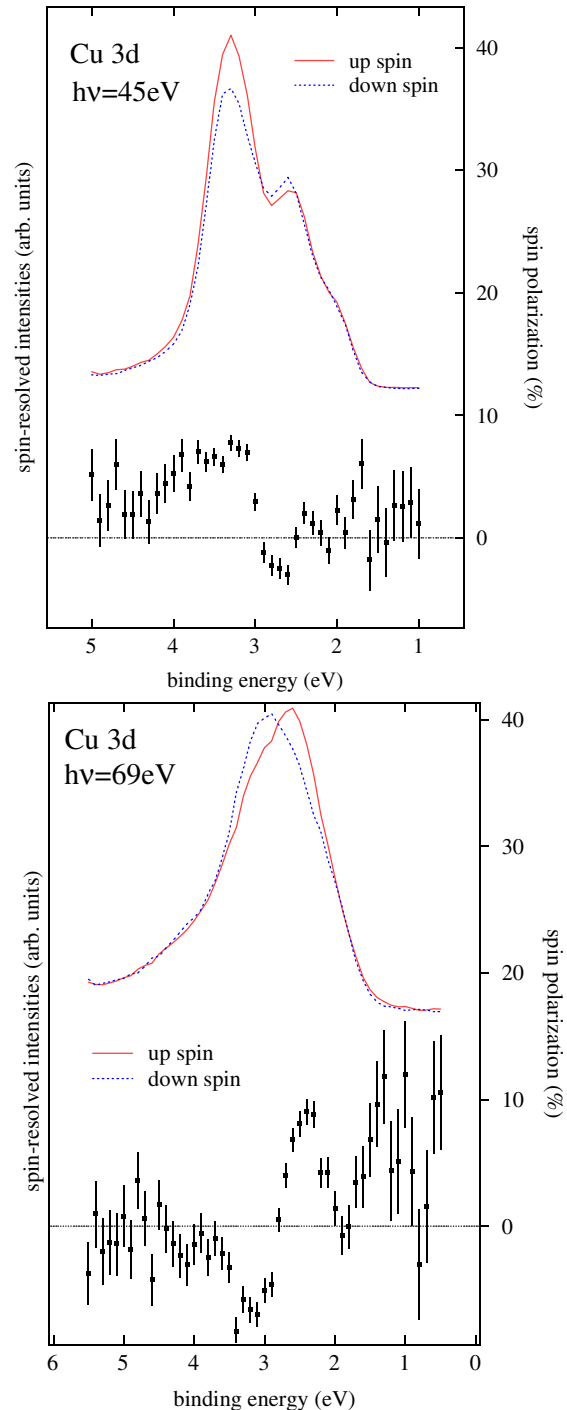
* akiok@hiroshima-u.ac.jp

Fig.1 SARPES spectra of Cu(001) taken at $h\nu$=45eV (a) and $h\nu$=69eV (b).

Spin-dependent interface electronic states of fcc Fe/Co(001)

Akio KIMURA[1*], Nozomu KAMAKURA[1], Kei HAYASHI[1],
Ayumi HARASAWA[1], and Akito KAKIZAKI[1]

[1]Tsukuba Branch of ISSP, The University of Tokyo, Tsukuba, Ibaraki 305-0801, Japan

Fe thin film on noble metal surface shows a variety of magnetic properties and many experimental studies have been devoted to clarifying the relationship between magnetism and electronic structure. It is known that the Fe thin film grown on Cu(001) forms a face-centered tetragonal (fct) structure with film thickness less than 5 monolayers (ML) and fcc structure with film thickness more than 5ML [1]. The ferromagnetism of fct Fe/Cu(001) has been explained by the large distance between Fe atoms along the direction normal to the surface [1]. A very similar structural character has been found for the room temperature growth of the Fe film on fcc Co(001) surface by low energy electron diffraction (LEED), and from analogy with the Cu case it has been suggested that the growth is very similar, in particular the presence of fct and fcc Fe below and above 5ML, respectively [2]. The magnetic properties are a little different from Fe/Cu(001) in the thickness range 5-11ML. O'Brien et al. have observed the small X-ray magnetic circular dichroism (XMCD) signal in fcc/Co(001) in the 5-11ML range at R.T. [2], To clarify the spin dependent surface and interface electronic states of fct and fcc Fe/Co(001), we have carried out the spin polarized photoemission spectroscopy of Fe and Co 3p core level.

The experiment was done at BL-19A, which is equipped with an angle-resolved spectrometer and a Mott polarimeter for photoelectron spin analysis. Base pressure of the ultrahigh-vacuum system was 1×10^{-10} Torr. The direction of the sample magnetization was <110>, which was parallel to the sample surface. The photoelectrons emitted normal to the sample surface were collected with the angle of incident light at 20° at R.T..

Fig.1 shows the spin resolved Fe 3p and Co 3p core level photoemission spectra of 0.9ML Fe/Co(001). The peak structure of the minority spin photoelectron spectrum is located at lower binding energy than that of the majority spin spectrum for both of the Fe and Co 3p core levels. It is known that the energy splitting between the majority and minority spin spectra is caused by the exchange coupling between the core hole spin and the 3d electron spin, which is related to the 3d spin magnetic moment. The result suggests that the Fe 3d derived spin magnetic moment is aligned parallel to that of the Co 3d state. It is evaluated that the energy splitting of the Fe 3p core level photoemission spectra is 0.8eV, which is larger than the reported value of the bcc Fe (~0.5eV) [3]. This large exchange splitting is consistent with the large exchange splitting in the Δ_5 band measured by the spin and angle resolved photoemission spectroscopy [4]. The corresponding energy splitting of 6.6ML Fe/Co(001) is

found to be much smaller (0.25eV). This is consistent with the result of the small XMCD asymmetry for the 5-11ML fcc Fe/Co(001) observed by O'Brien et al. In an analogical way to the case of Fe/Cu(001), we speculate that the topmost 2 layers show the ferromagnetism, whereas the bulk layers (below top 2 layers) show no net magnetic moment due to the formation of the antiferromagnetic or para-magnetic structure. This speculation is supported by the reduced energy splitting but finite spin polarization still found for 6.6ML Fe/Co(001).
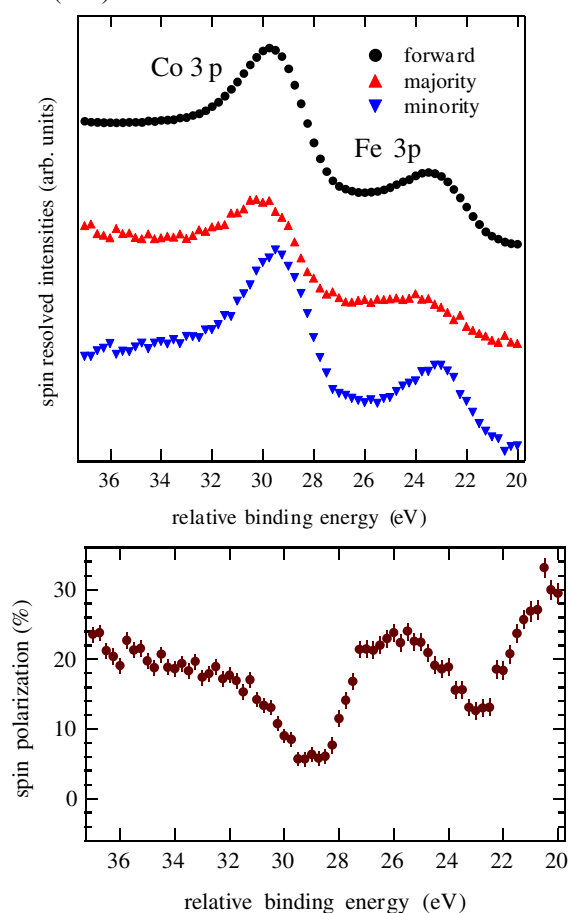

Fig.1 (a) Spin polarized Fe 3p and Co 3p photoemission spectra (a) and its spin polarization (b) of 0.9ML Fe/Co(001).

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* akiok@hiroshima-u.ac.jp

Angle resolved photoemission study of CrP(100)

Akio KIMURA[1*], Yoshio TAKAICHI[1], Atsushi MORIHARA[1], Seiichi WATANABE[1],
Yukiharu TAKEDA[1], Hitoshi SATO[1], Kenya SHIMADA[2], Masaki TANIGUCHI[1],
Atsushi FUJIMORI[3], Tatsuhiro NOZUE[4], Takashi KAMIMURA[4]

[1]Graduate School of Science, Hiroshima Univ., Higashi-Hiroshima 739-8526, Japan
[2]Hiroshima Synchrotron Radiation Center, Hiroshima Univ., Higashi-Hiroshima 739-8526, Japan
[3]Department of Complexing Science and Engineering, Univ. of Tokyo, Bunkyo-ku 113-0033, Japan
[4]Department of Physics, Tohoku Univ., Sendai 980-8578, Japan

It is well known that 3d transition metal monopnictides show various structural and magnetic properties. Among them, some compounds show structural phase transitions between NiAs-type structure to orthorhombic MnP type structure. The structural properties have been considered to be related to the magnetic properties. The present study is devoted to the Pauli paramagnetic compound CrP, which forms the MnP type crystal structure as shown in Fig.1(a). Recently, high quality single crystal of CrP has been successfully grown by a chemical vapour transport technique [1], which makes possible to observe the de Haas-van Alphen (dHvA) effect. Ten branches of dHvA frequency in the (010) plane have been found in the dHvA effect measurement. These branches are partially explained by the calculated Fermi surface. The electronic structures related to their magnetism and the structural phase transition are needed to be investigated. In order to study the whole features of the valence band electronic states, the angle-resolved photoemission was carried out for the single crystalline CrP(100).

The experiment was done at BL-18A. The clean surface was obtained by the repeated cycles of Ar ion bombardment and annealing up to 800K. The angle resolved photoemission spectra were measured at hv=21.2eV on the $\Gamma(X)$-Y(S) and $\Gamma(X)$-Z(U) planes in the orthorhombic Brillouin zone as shown in Fig.1 (b). Besides the spectra along Γ-X axis changing the incident photon energy was likewise measured. Fig.2 shows the experimental energy band structure as a function of a parallel component along the [100] direction of the wave vector ($k_{//}$), corresponding to the $\Gamma(X)$-Z(U) direction in the Brillouin zone. The normal emission spectrum excited by the photon energy of 21.2eV shows the structures just below E_F and $E_B = 3.8eV$ and the small hump around 7eV, which are recognized at $k_{//} = 0$ (Å^{-1}) in Fig.2. With increasing the emission angle, the structure around 3.8eV at $k_{//} = 0$ (Å^{-1}) becomes broader and separates each other as clearly observed in the spectra above 30° ($k_{//} > 0.5$Å^{-1}). The weak structure at E_B=7eV at $k_{//} = 0$ (Å^{-1}) shifts toward the lower binding energy with increasing the emission angle up to 26° ($k_{//} \sim 0.5$Å^{-1}) and again go back toward the higher binding energy. Although the sharp structure just below E_F seems to stay at the same E_B at any emission angles, the intensity of this

peak is gradually suppressed (*not shown*). Comparing the experimental energy band structure with those calculated by LMTO method, we have found that the experimentally observed feature of the structure for Cr3d-P3p bonding state is well explained by the calculation.
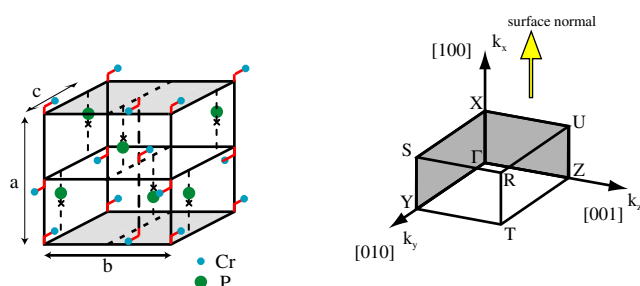

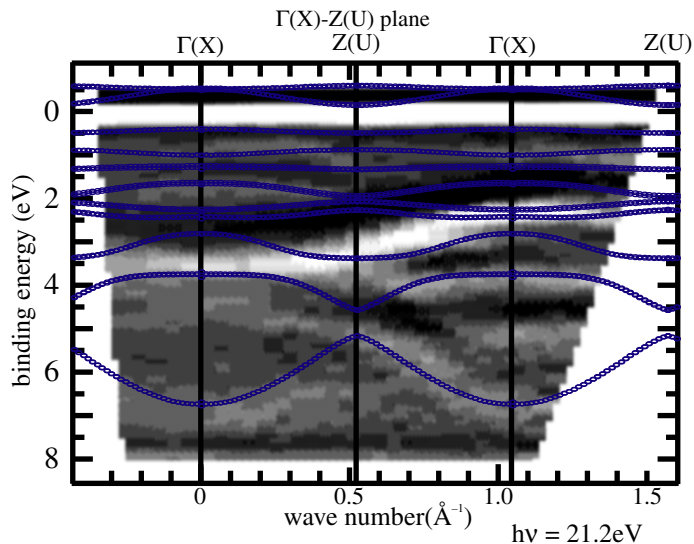Fig.1 (a) Crystal structure of CrP. (b) Orthorhombic Brillouin zone of CrP.

Fig.2 Experimental band structure of CrP(100) in $\Gamma(X)$-Z(U) plane in the orthorhombic Brillouin zone. The theoretical band structures calculated by LMTO method along X-U line are also shown for comparison.

References

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* akiok@hiroshima-u.ac.jp

Angle-resolved photoemission study of ordered CoPt₃(001)

Akio KIMURA[1*], Ki Seok AN[1], Ayumi HARASAWA[1], and Akito KAKIZAKI[1]

[1]Tsukuba Branch of ISSP, The University of Tokyo, Tsukuba, Ibaraki 305-0801, Japan

It is well known that ordered transition metal (TM)-platinum alloys show various magnetic properties. For example, the magnetic structure varies among MPt₃ (M=V, Cr, Mn, Fe and Co) as shown in Table. I. In order to clarify the origin of the variety of the magnetic structures, their electronic structures should be understood. Among them, CoPt₃ forms cubic $L1_2$ structure and ferromagnetic structure below a Curie temperature of 290K. In this report, we have successfully obtained 1x1 clean surface of the single crystalline CoPt₃(001) and performed an angle resolved ultraviolet photoemission spectroscopy (ARUPS). The experiment was carried out at BL-18A of Photon Factory, KEK. The clean surface was obtained by the repeated cycles of Ar ion bombardment and annealing up to 510K, which is below the critical temperature of the order-disorder structural phase transition. Sharp 1x1 LEED pattern was obtained after the procedure as shown in Fig.1. The ARUPES spectra were taken at the photon energy (hν) of 20-150eV with a normal emission configuration. Here, the normal emission spectra represent the electronic states along Γ-X-Γ direction in the cubic Brillouin zone.

	VPt₃	CrPt₃	MnPt₃	FePt₃	CoPt₃
magnetic structure	Ferri	Ferri	Ferro	Antiferro	Ferro

Table I. Magnetic structures of MPt₃ alloys (M=V, Cr, Mn, Fe, Co).
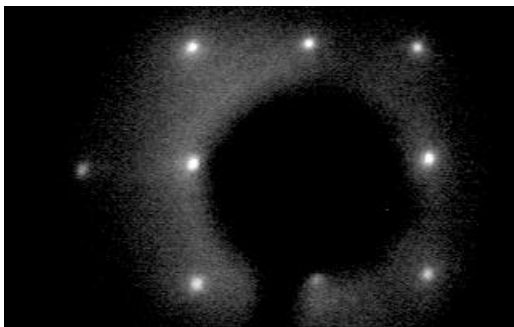

Fig.1. LEED pattern of the CoPt₃(001) surface.

The angle integrated photoemission spectra are measured for hν=46-130eV (*not shown*). It is known that the photo-ionization cross section of Pt 5d state is several times larger than that of Co 3d state for the photon energy range of 20-60eV, wheras the cross section of Pt 5d state drops dramatically around hν=100eV (Cooper-minimum). The angle-integrated photoemission spectrum at hν=46eV

(Pt 5d) shows the structures at E_B=0.3, 2.6, 5.5eV. The structure near E_F grows with increasing photon energy up to 130eV, where the photo-ionization cross section of the Co 3d state is more than 10 times larger than that of the Pt 5d state. The band structure calculation shows that the Pt 5d state is spread over a wide energy from E_F to 7eV, which is consistent with our experimental result at hν=46eV, for example. Comparing with the results of the band structure calculation, the observed sharp structure of the spectrum taken at hν=130eV can be assigned to the Co 3d minority spin state. The angle resolved spectrum taken at hν=46eV shows the structures at E_B=0.3, 2.5 and 5.5eV as shown in Fig.2. The small sharp structure observed just below E_F diminishes for the spectra taken at hν above 60 eV. The other structures at 2.5 and 5.5 eV does not show a remarkable dispersion. Such a dispersion-less feature will be discussed in a forthcoming paper. To clarify the spin dependent feature of the experimental band structure, the spin- and angle- resolved photoemission spectroscopy will be performed in near future.
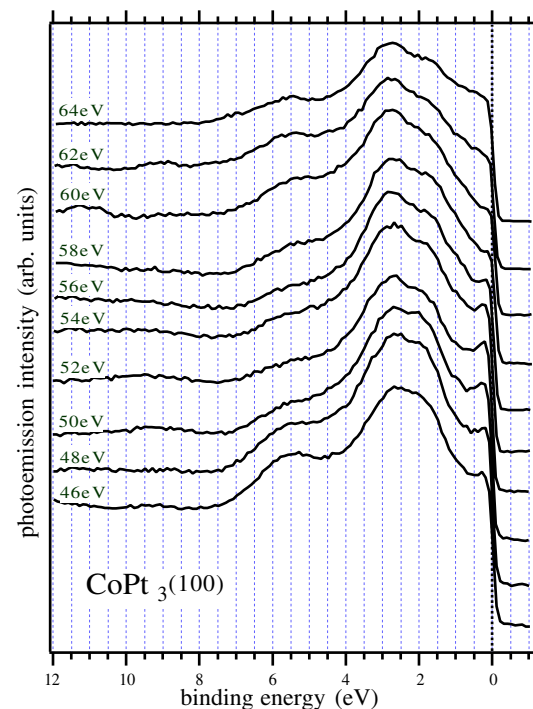

Fig.2 Angle-resolved photoemission spectra of CoPt₃(001) for hν=46-64eV.

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* akiok@hiroshima-u.ac.jp

Magnetic circular dichroism of resonant X-ray emission for transition metals and rare-earth metals

Yasuhiro TAKAYAMA[1*], Motoki SHINODA[1], Chol LEE[1], Kenji OBU[1], Hidetsugu SHIOZAWA[1]
Hiroyoshi ISHII[1], Tsuneaki MIYAHARA[1], Jun OKAMOTO[2]
[1]Tokyo Metropolitan Univ., 1-1, Minamiohsawa, Hachioji-shi, Tokyo 192-0397, Japan
[2]JAERI, 1-1-1, Mikazuki-cho, Sayo-gun, Hyogo 679-5148, Japan

Introduction

Measurement of the magnetic circular dichroism (MCD) of x-ray absorption has been a powerful technique to study magnetism. Recently, some experiments of measuring the MCD of x-ray emission have been reported in soft and hard x-ray regions. In VUV region, however, only a few experiments of the resonant x-ray emission and no experiment for its MCD have been performed. In this study, we have developed the experiments of the x-ray emission spectroscopy in VUV region. For this purpose, we have measured 3p-3d and 4d-4f resonant x-ray emission for transition metals and rare-earth metals, respectively.

Experimental

The experiment was performed at a helical undulator beamline BL-28A. The detail of the instrument was explained in the reference [1]. The instrument was composed of a sample chamber and a spectrometer. The energy resolution of the spectrometer was about 0.14 eV and 0.40 eV for the photon energies of 60 eV and 120 eV, respectively. By reversing the magnetic field applied to the sample, MCD signal of the x-ray emission was observed. The total accumulation time for an excitation energy was about 3 hours.

Result and Discussions

Figure 1 shows the x-ray emission spectra of Cobalt metal for the excitation energies of 60.8 eV (A), 61.6 eV (B), 62.3 eV (C) and 63.1 eV (D). The energies of 60.8 eV and 63.1 eV are below and above the threshold of 3p-3d excitation, respectively. Energy Shift is defined as the subtraction of the energy of the incident photon from that of the emitted photon. A sharp peak and a broad peak of the Raman scattering were found at the energy shift of -0.6 eV and -3.9 eV, respectively. The origin of the broad peak is assumed to be the excitation to the non-bonding final state of the $3d^7$ and $3d^8$ configurations. A broad peak was also found in the x-ray emission spectra of Nickel metal at the energy shift of -4.6 eV, which may be assigned as the non-bonding final state of $3d^8$ configuration. No clear sharp peak, however, was observed in the x-ray emission spectra of Nickel. Figure 2 shows the x-ray emission spectra and their MCD for Terbium metal. We changed the excitation energies between 140.4 eV (a) and 153.9 eV (h). The excitation energy between 143.9 eV (b) and 147.5 eV (e) (149.6 eV (f) and 153.9 eV (h)) correspond to the 4d-4f resonant

excitation to the pre-threshold (giant) peaks of the x-ray absorption spectra. At the energy shift of about -22 eV, a sharp peak of the Raman scattering was observed and the intensity of the peak resonantly enhanced for the excitation energy of 143.9 eV (b). A large negative MCD was also found in this peak. The peak is originated from the excitation of the electron in the 5p state to the 4f state. Another peak was found at the energy shift of about -4 eV. This peak is originated from the spin-flipped final state. These peaks were also observed in the spectra of Gadolinium, Dysprosium and Holmium metals, and the qualitative features of the spectra were very similar for these rare-earth metals.
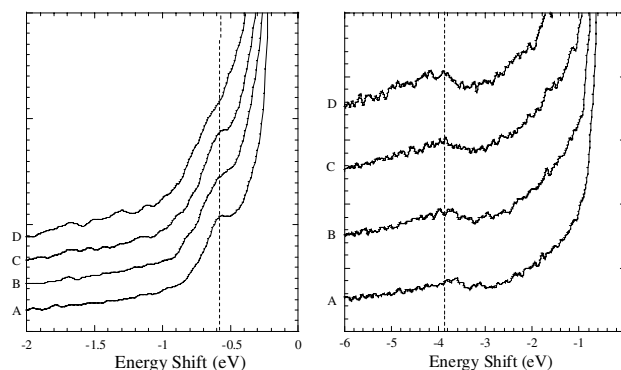

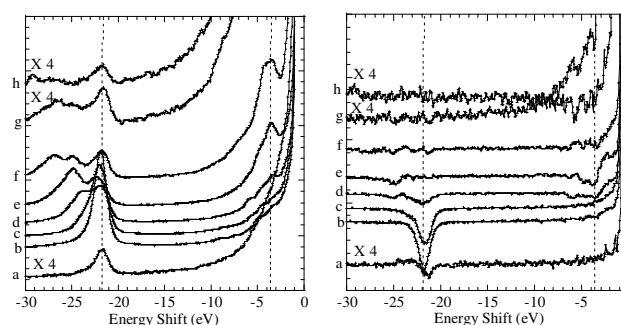Figure 1: X-ray emission spectra for Cobalt metal.

Figure 2: X-ray emission spectra (left) and their MCD (right) for Terbium metal.

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[*]takayama@phys.metro-u.ac.jp

Soft X-ray magnetic circular dichroism on Fe/Tb multilayer films

Katsuyoshi TAKANO, Miki FURUHATA, Kazuhiro IKEUCHI, Hiroshi SAKURAI,
Fumitake ITOH, Hiromi OIKE

Department of Electronic Engineering, Gunma Univ., 1-5-1 Tenjin-cho, Gunma, 376-8515, Japan

Fe/Tb multilayers were prepared on Al foil by a dual-type radio frequency sputtering method (Table 1. A) and MBE at the SVBL, Gunma University (Table 1. B~D). The sample A~D have almost same Tb thickness with different Fe thickness. The sample A has almost the same Fe thickness and Tb thickness as the sample B, but has rough interface.

Table 1

Sample	Fe [nm]	Tb [nm]	Stack [No.]
A	0.7	0.5	25
B	1.0	0.4	125
C	1.9	0.5	125
D	5.7	0.8	125

The Soft X-ray Magnetic Circular Dichroism (SXMCD) was measured on the beam line AR-NE1B of KEK, Japan. The SXMCD spectra at both the Fe $L_{2,3}$-edge and the Tb $M_{4,5}$-edge were taken with the total electron yield method under the magnetic field applied perpendicular to the sample plane of 1 T at room temperature. The SXMCD spectra were normalized with the "edge-jump" of the X-ray absorption spectra. Figure 1 shows the SXMCD spectra of the Fe/Tb multilayers. In the sample B~D, SXMCD signals at the Fe L_3-edge are negative and those at the Tb M_5-edge are positive. This shows clearly the magnetic moment of Fe align to the magnetic field and the magnetic moments of Tb are coupled ferri-magnetically with Fe moments. This is consistent with the result by hard X-ray MCD.[1] However, The SXMCD signals at both the Fe L_3-edge and Tb M_5-edge are negative in sample A. Namely, the Fe and Tb moment are coupling ferro-magnetically in case of thin Tb layer.

Figure 2 shows the individual m_{orb} (a) and m_{spin} (b) of the Fe (solid circle) and Tb (open circle) that obtained from the magneto-optical sum rule.[2][3] We used the values of 6.61 and 8 for as a number of Fe $3d$ [4] and Tb $4f$, respectively. The m_{orb} and m_{spin} of Fe in these samples is small in compared to the bulk Fe, $0.085\mu_B$ and $1.98\mu_B$.[4] The m_{orb} of the Fe almost zero in the sample B~D. But in the sample A that has $0.032\mu_B$. The m_{spin} of Fe and Tb decrease with decreasing the Fe thickness in the sample B~D. In sample A, the m_{spin} of Tb moment is enhanced and the m_{spin} of Fe moment is suppressed.

We suggest the following model; In the B~D, the Fe moments have stronger in-plane anisotropy with decreasing the Fe thickness. The Tb moment also cant to in-plane keeping the ferri-magnetically coupling with the

Fe moments. Then the m_{spin} of Fe and Tb decrease with decreasing the Fe thickness. In the sample A with rough interface, the Tb moments cant to the applied field, but Fe moments have still in plane anisotropy. Then out of plane contribution is enhanced in Tb moment and is suppressed in Fe moment. A semi-quantitative simulation is required for analysis of this phenomenon.
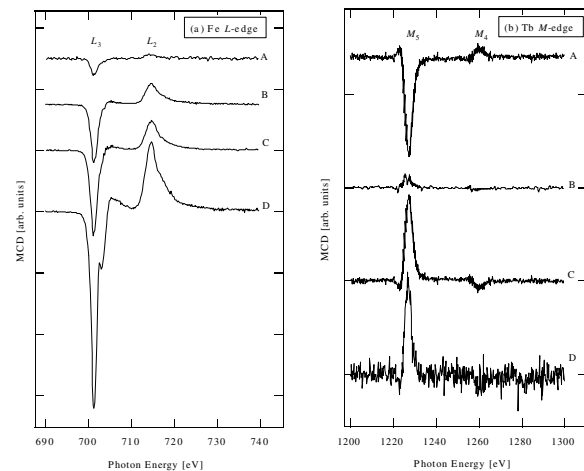

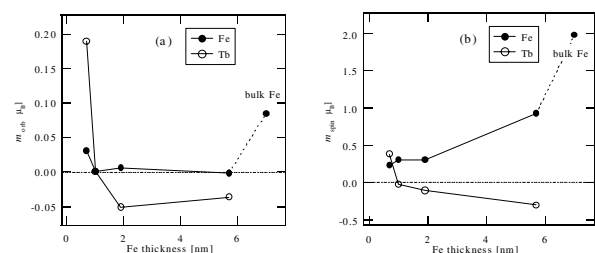Figure 1. The SXMCD spectra at Fe $L_{2,3}$-edge (a) and Tb $M_{4,5}$-edge (b) at 298K.

Figure 2. m_{orb} (a) and m_{spin} (b) of Fe (solid circle) and Tb (open circle).

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* ktakano@el.gunma-u.ac.jp

Magnetization process of Fe/Tb multilayer films by MCD study

Katsuyoshi TAKANO, Kazuhiro IKEUCHI, Hiroshi SAKURAI,
Fumitake ITOH, Hiromi OIKE

Department of Electronic Engineering, Gunma Univ., 1-5-1 Tenjin-cho, Gunma, 376-8515, Japan

The Fe/Tb multilayer of the composition [Fe 121 nm / Tb 156 nm] × 25 were prepared on Al foil by a dual-type radio frequency sputtering method.

The XMCD measurements were performed on the beam line PF-BL-28B of KEK, Japan. The examples of the XMCD spectra at both Fe K-edge and Tb L_3-edge in the magnetic field of 0.62 T at room temperature are shown in Fig.1. The XMCD spectra were normalized with the total thickness of each element, which was estimated from the normal absorption spectra. And those were corrected with the degree of circular polarization of the incidence X-ray. The magnitude of XMCD was estimated with integrating the energy range from 7.107 eV to 7.109 eV in Fe K-edge and the energy range from 7.511 eV to 7.521 eV Tb L_3-edge, as shown Fig.1(a), (b). The sign of XMCD of Tb is opposite to Fe. This shows clearly the magnetic moments of Tb in the multilayer are coupled ferri-magnetically with Fe moments in this Fe/Tb sample.

In order to measure the magnetization process of each element separately, we have measured the magnetic field dependence of the XMCD intensity. [1],[2] The sample was at first demagnetized. Then the XMCD intensity was measured at a given magnetic field (reversing up and down). This measurement was repeated by stepwise increasing the magnetic field from 0.02 T to 0.62 T. Thus obtained information corresponded to the initial magnetization of each element in the M-H curve. [2]

The results are shown in Fig.2 as a function of temperature. The magnitude of XMCD in both elements was normalized with that in bulk Fe at 0.62T, 298K and bulk Tb at 0.62T, 200K, respectively. We should note the variety of XMCD with signs. Above T=100 K, both the magnitude of Fe K-edge and Tb L_3-edge increase proportional up to H=0.15 T. This suggests both Fe and Tb moments increase with increasing the magnetic field, keeping the ferri-magnetic coupling. Below at T=150K, the magnitude of Fe increases, while that of Tb decreases with increasing the magnetic field.

Below 150 K, the variations of XMCD intensity can be explained by a twisted model; The magnetic moments of Fe and Tb align anti-parallel in the low field. But the magnetic moment of Tb begins to turn to the applied field, keeping the Fe moment constant.
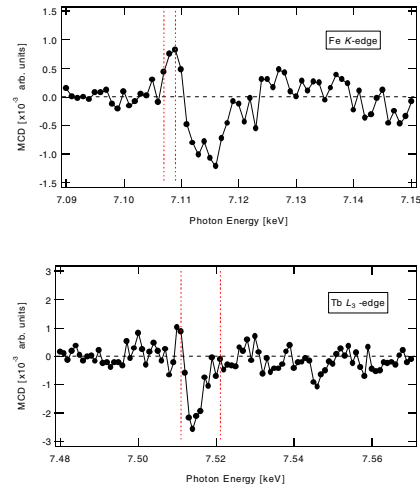

Fig. 1. An example of the XMCD spectra at Fe K-edge (a) and Tb L_3-edge (b) in the field of 0.62 T at 298K.
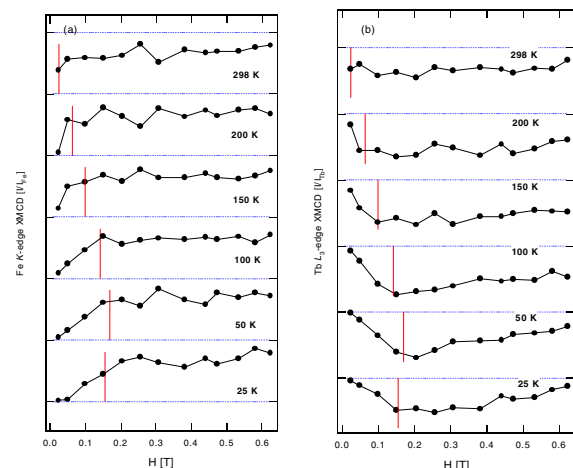

Fig. 2. Field dependence of the Fe K-edge (a) and the Tb L_3-edge (b) XMCD integrated intensity at 298K, 200K 150K, 100K, 50K, and 25K, respectively. Longitudinal lines denote the cohesive field in the M-H curve.

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* ktakano@el.gunma-u.ac.jp

Resonant photoemission spectroscopy of CeFe$_4$P$_{12}$ and CeRu$_4$Sb$_{12}$

Hiroyoshi ISHII*, Tsuneaki MIYAHARA, Yasuhiro TAKAYAMA, Hideo OTSUBO,
Kenji OBU, Chol LEE, Hidetsugu SHIOZAWA, Tatsuma D. MATSUDA,
Yuji AOKI, Hitoshi SUGAWARA and Hideyuki SATO
Tokyo Metropolitan University, Hachioji-shi, Tokyo 192-0397, Japan

Introduction

Ternary intermetallic compounds RT$_4$X$_{12}$ (R= rare earth element, T= Fe, Ru, Os and X= P, Sb) with the filled skutterudite structure exhibit various interesting properties. According to the measurements on a high quality single crystal [1, 2], CeFe$_4$P$_{12}$ shows the complex temperature dependence of resistivity unexpected for a simple single-gap semiconductor; CeRu$_4$Sb$_{12}$ was thought to be a Kondo system with T_K=100 K. We investigated the electronic states of CeFe$_4$P$_{12}$ and CeRu$_4$Sb$_{12}$ by the Ce 3d-4f and Ce 4d-4f resolution resonant photoemission spectroscopy.

Experimental

The photoemission experiments were performed using synchrotron radiation at the beam lines BL-11D and BL-2C of the Photon Factory, High Energy Accelerator Research Organization (KEK). The instrumental resolutions were 65 meV and 250 meV for the 4d-4f resonance and the 3d-4f resonant photoemission, respectively.

Results and discussion

Figure 1 shows the Ce 4f spectra of CeFe$_4$P$_{12}$ measured by the Ce 3d-4f and Ce 4d-4f resonant photoemission. These spectra were obtained by subtracting the respective resonance minimum spectra from the respective resonance maximum spectra in the Ce 3d or 4d excitation regions. In the 4f spectra, the peaks located at ~2.6 eV and ~0.5 eV correspond to the f^0 and f^1 peaks, respectively.
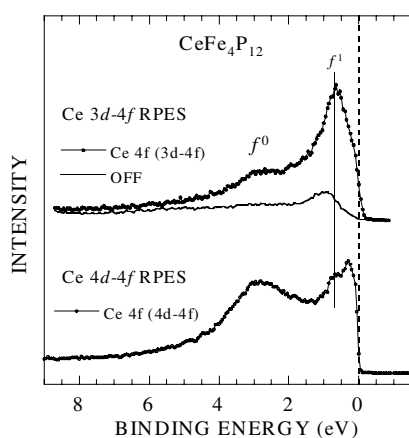
In the Ce 4f spectrum obtained by the 3d-4f resonant photoemission with a high bulk sensitivity, the intensity of the f^1 peak is very strong. This fact indicates the strong hybridization between the Ce 4f and the valence band states. The f^1 peak obtained by the Ce 3d-4f resonance was observed as a peak structure at 0.7 eV. On the other hand, the f^1 peak measured by the Ce 4d-4f resonance was observed as a shoulder at 0.7 eV. This different in spectral shape may due to the strong hybridization between the Ce 4f state and the Fe 3d band.

Figure 2 shows the Ce 4f spectra of CeRu$_4$Sb$_{12}$ measured by the Ce 3d-4f and Ce 4d-4f resonant photoemission. In the both spectra, the $f_{5/2}^1$ peak located just below E_F was observed as a shoulder structure. According to the experimental and theoretical results of the Ce 4f spectrum of a Kondo system [3], the spectral shape of the $f_{5/2}^1$ peak ascribed to the tail of the Kondo resonance peak varies from a shoulder to a prominent peak with increasing T_K. The shoulder structure for CeRu$_4$Sb$_{12}$ is similar to the feature observed in the very low-T_K Ce system. From that point of view, CeRu$_4$Sb$_{12}$ is a low-T_K system.

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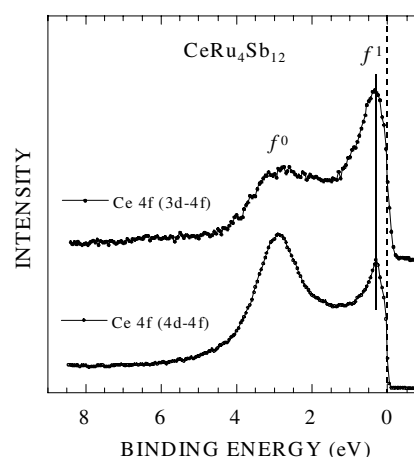[3] F. Patthey *et al.*, Phys. Rev. **B 42** (1990) 8864.

Figure 1: Ce 4f spectra of CeFe$_4$P$_{12}$ obtained by the Ce 3d-4f and 4d-4f resonant photoemission.

Figure 2: Ce 4f spectra of CeRu$_4$Sb$_{12}$ obtained by the Ce 3d-4f and 4d-4f resonant photoemission.

* ishii@comp.metro-u.ac.jp

Orbital- and spin- magnetic form factor of ferromagnetic YTiO$_3$ measured by the X-ray magnetic diffraction

Masahisa ITO*[1], Hiromichi ADACHI[2], Hironori NAKAO[3], Youichi MURAKAMI[3],
Yasujiro TAGUCHI[4], Yoshinori TOKURA[4], Kenichi KATO[5], Eiji NISHIBORI[5],
Masaki TAKATA[5], Makoto SAKATA[5], Hayato MIYAGAWA[6], Susumu NANAO[6],
Hiroshi MARUYAMA[7], Etuo ARAKAWA[8] and Kazumichi NAMIKAWA[8]

[1]Gunma University, Aramaki 4-2, Maebashi, Gunma 371-8510, Japan
[2]KEK-PF, Oho 1-1,Tsukuba, Ibaraki 305-0801, Japan
[3]Graduate School of Science, Tohoku University, Aramaki ,Aoba-ku, Sendai, 980-8578, Japan
[4]School of Engineering, The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan
[5]School of Engineering, Nagoya University, Furoucho , Chikusa-ku, Nagoya 464-0814, Japan
[6]IIS, The University of Tokyo, Komaba 4-6-1, Meguro-ku, Tokyo 153-8505, Japan
[7]Faculty of Science, Hiroshima University, Kagamiyama 1-3-1, Higashihiroshima 739-8526, Japan
[8]Faculty of Education, Tokyo Gakugei University, Nukuikita 4-1-1, Koganei, Tokyo 184-8501, Japan

YTiO$_3$ is one of the orbital ordering systems of 3d electrons. The 3d electronic configuration of Ti^{3+} is (t2g)^1. The orbital ordering of this compound has been studied theoretically and experimentally. The experimental models of the ordered orbitals were based on the assumption that the orbital moments are quenched[1,2]. In this study we made the X-ray magnetic diffraction (XMD) measurement of ferromagnetic YTiO$_3$ in order to measure the orbital (L)- and the spin (S)-magnetic form factor utilizing the ability of the XMD of LS separation.

The XMD measurement was made using a four-circle diffractometer with an electromagnet and a refrigerator of liquid-He flowing type. Magnetic field strength was 3 kOe and the temperature of the specimen was 5 K. This compound is ferromagnetic below 28K. The easy magnetization axis is [001]. Magnetization measurement showed that the 3kOe was enough to saturate the magnetization of the specimen along the [001] axis.

The reflection plane of the specimen crystal was (068). The scattering angle at the specimen was 90 degree. We adopted two experimental configurations. First, the magnetic field direction was aligned along the incident X-rays, which was almost the same direction as the [001] axis. This configuration made us observe the orbital-magnetic form factor selectively at the reciprocal lattice point, 068. Second, the magnetic field was applied parallel to the diffracted x-ray beam and, at the same time, the specimen crystal was turned upside down, such that the reflection plane was also (068) and the magnetic field was parallel to the [001] axis. This configuration made us observe the total(spin+orbital) magnetic form factor at 068. The magnetic form factor was obtained by measuring the change in the diffraction intensity caused by reversing the magnetic field direction.

The obtained orbital-magnetic form factor is shown as a rhombus in Fig. 1. The orbital magnetic moment was estimated, assuming the dipole approximation curve (dotted lines), to be 0.03±0.1μ$_B$, and is shown in Fig. 1 as a solid circle. The open circle in Fig. 1 is the measured magnetic moment of the specimen crystal. From Fig. 1 it is seen that the orbital contribution to the magnetic moment would be very small.

By combining the orbital- and the total magnetic form factors we obtained the spin- magnetic form factor of 068, and is shown in Fig. 2 as a solid rhombus. In Fig. 2 the spin-magnetic form factor of 068 is compared with those of 00l (l=6-12), which were previously measured[3]. Anisotropy in the spatial distribution of the spin magnetic moments might be reflected in Fig. 2. Double circles and a double rhombus are the calculated spin magnetic form factors using the wave functions in [1]. Despite the discrepancy between the experiment and the calculation, both data show similar tendency.
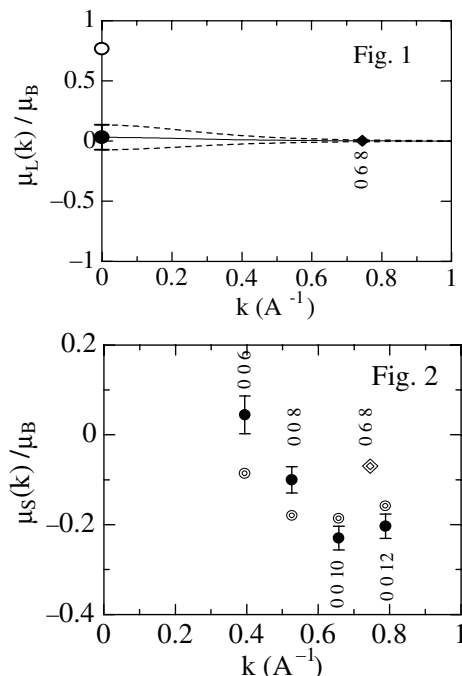
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* itom@fs.aramaki.gunma-u.ac.jp

L_3-edge XAFS measurements of valence fluctuating Eu compounds

Akihiro Mitsuda*[1], Shuichi Fukuda[1], Yuji Nakanuma[1], Tsuyoshi Ikeno[1], Yosikazu Isikawa[1], Junji Sakurai[1] and Tsunehiro Tanaka[2]

[1]Department of Physics, Toyama University, 3190 Gofuku, Toyama 930-8555, Japan
[2]Department of Molecular Engineering, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan

Introduction

It is known that some Eu compounds show a valence fluctuation like Ce and Yb compounds. The valence fluctuation in Eu compounds takes place between non-magnetic Eu^{3+} and Eu^{2+} with a localized moment of $7\mu_B$. One of great interest in the valence fluctuation in Eu compounds is that the mean Eu valence strongly depends on temperature, magnetic field and pressure[1,2]. In this study, we take notice of $EuCu_2(Si_xGe_{1-x})_2$ system which was reported to exhibit a Kondo-lattice type state by Levin et al. for the first time [3]. Recently, heavy fermion behavior has been reported by Hossain et al. [4]. In order to discuss a correlation between such phenomena and the valence, we have investigated the mean Eu valence as a function of temperature by measuring L_3-edge XAFS.

Experimental

The polycrystalline samples were prepared by arc-melting under argon atmosphere and subsequent annealing in an evacuated quartz tube at 1173 K for 1 week. The XAFS measurements at the Eu L_3 edge were performed at BL-9A beamline of KEK Photon Factory using a Si(111) double crystal monochromator in the temperature range from 10 K and 300 K.

Results and discussion

All of the measured XAFS spectra at the Eu L_3 edge of the samples consist of two subspectra, the $(2p^5 4f^7 5d^*)$ and $(2p^5 4f^6 5d^*)$ final state components, as shown in Fig. 1. This directly indicates the valence fluctuating behavior. The spectra were analysed by fitting two sets of a Lorentzian and an arctangent-function. The mean valence is estimated from the relative intensity of the two subspectra. Figure 2 shows the mean valence of the samples as a function of temperature. For x 0.65, the valence shifts toward the Eu^{3+} state with decreasing temperature. For x=0.70-0.80, the T_0 means the temperature where magnetic susceptibility of the samples begins to deviate from a Curie-Weiss law. The valence at T_0 is found to be an almost common value of ~2.4, which appears to be a boundary between a non-magnetic Eu^{3+} and a magnetic Eu^{2+} characters. The valence at the lowest temperature has an intermediate value of 2.5-2.65. Similar behavior is observed also in $EuNi_2Si_2$, which has a large electronic specific heat coefficient of $\gamma \sim 100 mJ/K^2$ mol. The intermediate valence is possibly associated with the heavy fermion behavior.

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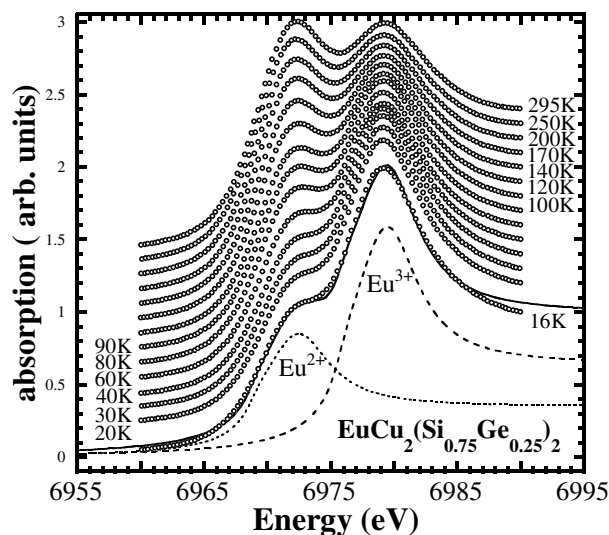[1] A. Mitsuda et al., Phys. Rev. B, **55**, 12474 (1997).

Fig. 1 The XAFS spectra at the Eu L_3-edge at various temperatures.
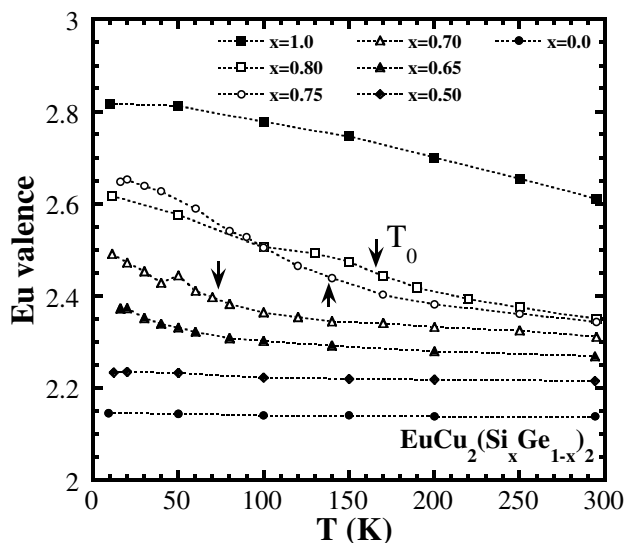

Fig. 2 Temperature dependence of the mean Eu valence.

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* a3da@sci.toyama-u.ac.jp

Resonant x-ray scattering study of NaV$_2$O$_5$ under high pressure

Kenji OHWADA[*1], Hironori NAKAO[2], Youichi MURAKAMI[2],
Yasuhiko FUJII[3], Masahiko ISOBE[3] and Yutaka UEDA[3]
[1]JAERI/SPring-8, Mikazuki-cho, Sayo-gun, Hyogo 679-5148, Japan
[2]Tohoku Univ., Aoba-ku, Sendai, Miyagi 980-8578, Japan
[3]ISSP Univ. of Tokyo, Kashiwa-no-ha, Kashiwa, Chiba 277-8581, Japan

Introduction

Devil's Flower has been reproduced in the Temperature-Pressure phase diagram of charge-lattice-spin coupled system NaV$_2$O$_5$ [1]. All of experimentally observed phases have $2a \times 2b \times Zc$ type superstructures and the corresponding wave number q_c (=1/Z, C_{q_c}-phase) sequences at several temperature and pressure ranges are well understood as the **Devil's Staircase** type sequence theoretically obtained from the ANNNI model [2]. The q_c sequences were directly determined by the synchrotron x-ray diffraction technique which well probes the lattice modulation but barely probes the charge modulation. It is not clear whether the charge modulation has the same q_cs observed in Ref. [1].

Experimental

To clarify the coupling of the two degree of freedom, charge and lattce, we have investigated the resonant x-ray scattering (RXS) at low temperature and high pressure around V K-edge (5.47 keV). The RXS well probes the charge modulation. Since the 5.47 keV x-ray cannnot through the diamond anvils, we have thus developed a new diamond anvil cell for RXS (RXS-DAC) as schematically shown in Fig. 1. 5.47 keV x-ray comes into and comes out from the sample chamber through the Be gasket. Single crystal of NaV$_2$O$_5$ and NaCl (for pressure marker) were enclosed with the n-i pentane 50:50 mixture for pressure transmitting media.
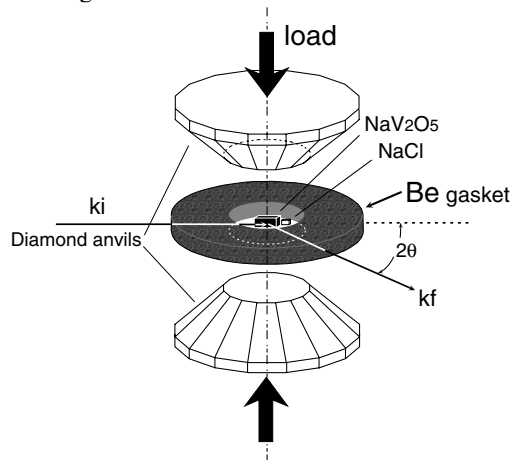

Figure 1: Schematical drawing of the RXS-DAC.

Result and discussion

Fig. 2 shows the energy scan at Q = (7.5 0.5 L) observed at 0.1 MPa (L=0.25, $C_{1\ 4}$-phase), 0.6 GPa (L=0.25, $C_{1\ 4}$-phase) and 1.2 GPa (L=0.0, C_0-phase) at 8K. Peaks around 5.468 keV (pre-edge) and 5.475 keV (main-edge) well reect the edge difference between V^{4+} and V^{5+} generated by the charge ordering. We also observed the similar energy prol e at (7.5 0 0.2) and nally conrmed that the charge modulation and the lattice modulation have the same q_cs. The intensity reduction at pre-edge (5.468 keV) may be caused by the geometical change around the V sites [3]. On the other hand, the main-edge peak intensity at 5.475 keV shows the pressure independence. This means that the charge order fully takes place in spite of the atomic shift suppression [1] under pressures.
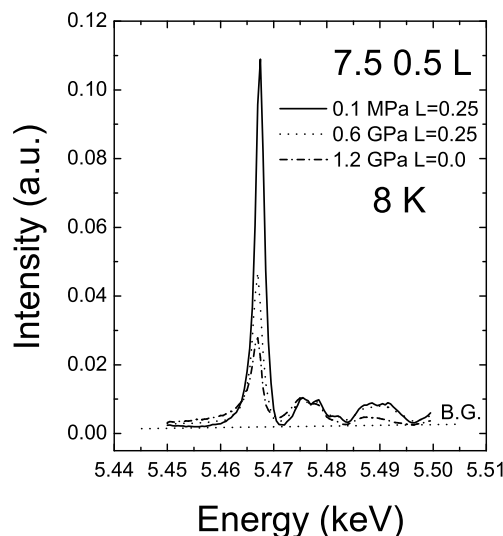

Figure 2: The energy scan at Q = (7.5 0.5 L) observed at 0.1 MPa (L=0.25, $C_{1\ 4}$-phase), 0.6 GPa (L=0.25, $C_{1\ 4}$-phase) and 1.2 GPa (L=0.0, C_0-phase) at 8K.

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*ohwada@spring8.or.jp

B *K* emission spectra for MgB_2 and $Mg_{0.8}Al_{0.2}B_2$

Noboru MIYATA*[1], Takashi IMAZONO[1], Mihiro YANAGIHARA[1], Makoto WATANABE[1],
Takahiro MURANAKA[2], Jun AKIMITSU[2]

[1]IMRAM, Tohoku University, Katahira, Aoba-ku, Sendai 980-8577, Japan
[2]Aoyama-Gakuin University, Chitosedai, Setagaya-ku, Tokyo 157-8572, Japan

Introduction

Recently, MgB_2 was shown to be a superconductor with Tc=39 K by Nagamatsu *et al* [1] . Since the discovery, the nature of the superconductivity in MgB_2 has been studied. The results suggest strongly that MgB_2 is a conventional BCS-type phonon-mediated superconductor. Within the related materials, Al-doped MgB_2 was one of the objects whose superconductivity was earlier estimated by theoretical and experimental aspects [2] . To confirm these results, soft-X-ray emission (SXE) spectroscopy is a useful method. Since the SXE spectrum reflects the partial density of states (PDOS) of the valence band, B *K* emission for MgB_2 shows the PDOS of the B $2p$ band. B $2p$ is a dominant component at the Fermi level, which is closely related with the Tc of superconductors. Thus B *K* emission spectra of MgB_2 and Al-doped MgB_2 ($Mg_{0.8}Al_{0.2}B_2$) provide much information of the superconductivity in MgB_2.

Experiments

The samples were sintered polycrystals of MgB_2 and $Mg_{0.8}Al_{0.2}B_2$. Phase purity and the Tc of the samples were estimated before the SXE measurements. X-ray diffraction patterns showed that all the samples were of a hexagonal phase with the lattice constants a=0.3086 nm and c=0.3524 nm for MgB_2 and slightly larger for $Mg_{0.8}Al_{0.2}B_2$. The temperature-dependent magnetization measurements showed that the Tc of the samples were 39 K for MgB_2 (x=0) and 29 K for $Mg_{0.8}Al_{0.2}B_2$, respectively. SXE experiment was performed at BL-16B. The FWHM of the incident SR soft X-ray at 191.1 eV was 0.5 eV, and of the spectrometer we used was 0.8 eV. Samples were filed in the preparation chamber before the measurements to remove surface contaminations.

Results and discussion

Figure 1 shows the B *K* emission spectra measured for MgB_2 and $Mg_{0.8}Al_{0.2}B_2$. The spectrum for MgB_2 (solid circles) has a main peak around 183 eV and Rayleigh scattering peak around 191eV. The spectral shape almost resembles the PDOS obtained by the band calculation of MgB_2. Compared with this spectrum, that for $Mg_{0.8}Al_{0.2}B_2$ (open circles) shifts about 0.3 eV towards the lower energy side.

The reason of the peak shift is explained as follows; B

$2p$ band, which is shown by the B *K* emission spectrum, can separate into σ and π bands. The σ band is pulled up by ionized Mg, which results in a hole-doping into the σ band. The peak of the B *K* emission spectrum of MgB_2 is contributed from the σ band around the *M* and *L* point in Brilluan zone, positioned about 2 eV below the Fermi level. The B-B in-plainer bonding is shortened by Al doping. It causes the σ bonding to be tight, and results in lowering of the σ band. This effect may cause the shift of the spectra qualitatively.
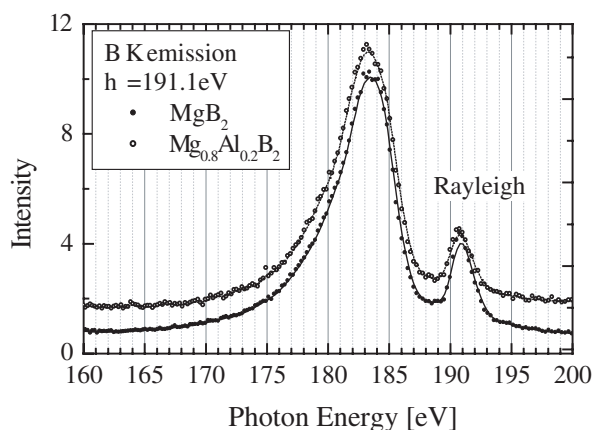

Figure 1: B *K* SXE spectra for MgB_2 and $Mg_{0.8}Al_{0.2}B_2$. The peak at about 191 eV in each spectrum is due to the elastic scattering of the incident soft X-rays.

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*nmiyata@mit.pref.miyagi.jp,
Present address: Industrial Technology Institute, Miyagi Prefectural Government, Akedori, Izumi-ku, Sendai 981-3206, Japan.

In-situ photoemission study of the room-temperature ferromagnetism in ZnGeP$_2$: Mn

Y. Ishida*, D. D. Sarma[1], K. Okazaki, J. Okabayashi, A. Fujimori,
G. A. Medvedkin[2], T. Ishibashi[3], and K.Sato[3]
Department of Physics, University of Tokyo, Tokyo 113-0033, Japan
[1]SSCU, Indian Institute of Science, Bangalore 560-012, India
[2]Ioffe Physico-Technical Institute, St. Petersburg 194021, Russia
[3]Tokyo University of Agriculture and Technology, Tokyo 183-8538, Japan

After the successful synthesis of III-V-based ferromagnetic diluted magnetic semiconductors (DMS or DFS), it is now crucial to increase the T_C above the room temperature (RT) for practical applications. There are several reports of RT-DFS such as TiO$_2$:Co, ZnO:Co, and ZnO:V. Among them is the intriguing report of the Mn incorporated II-IV-V$_2$-type chalcopyrite semiconductors CdGeP$_2$ and ZnGeP$_2$, which show ferromagnetism above 350 K [1]. High concentration of Mn ions are incorporated in the surface region by depositing Mn on the surface of ZnGeP$_2$ single crystals annealed at 400℃. Chemical reaction and the composition in the densely Mn-deposited surface region are still to be clarified.

In order to study the chemical and electronic structures of ZnGeP$_2$:Mn interface, we performed extensive *in-situ* photoemission measurements. Core-level and valence-band spectra were taken for various amounts of Mn deposition on the ZnGeP$_2$ surface. As the Mn was deposited, Zn signal quickly disappeared while the Ge and P were always present even after depositing the nominal Mn thickness of 500 A. The magnetization curve measured by SQUID for this 500 A Mn deposited surface showed a two component ferromagnetic behavior, one vanishing at 290 K, and the other showing ferromagnetism even above 375 K. The former component may be assigned to MnP (T_C = 290 K), while the latter is attributed to some ternary compound(s) of Mn, Ge, and P.

The valence band spectra showed a prominent Mn 3p-3d resonant peak up to the nominal Mn thickness of 30 A, while the Mn M$_{23}$VV Auger decay replaced the resonant behavior for further Mn deposition (Fig. 1). A clear Fermi edge was observed after 10 A Mn deposition, and its intensity was enhanced for further Mn deposition up to 100 A, beyond which both the ratio of the core-level intensities and the valence-band feature drastically changed. This indicates successive transitions from a DMS-like chemical state to other metallic compounds with Mn deposition on the ZnGeP$_2$:Mn interface.
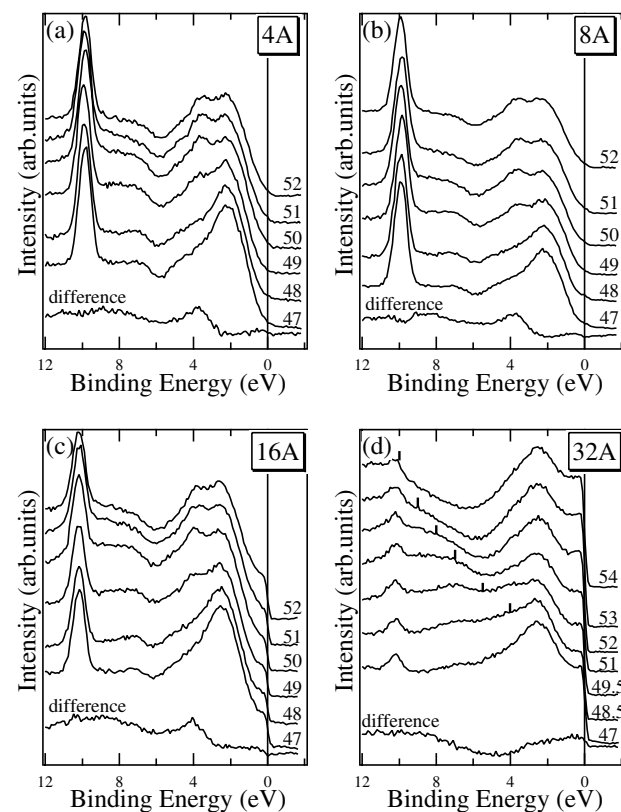

Fig. 1. Valence-band spectra of the nominal Mn thickness of 4, 8, 16, and 32 A in the Mn 3p-3d core excitation region. Every spectrum is normalized to the photon flux. The difference spectra are taken between on-resonance (hν =51eV) and off-resonance (hν =48eV). The difference specrta below 30 A Mn deposition represent the Mn 3d partial DOS. The vertical bars in (d) denote the Mn M$_{23}$VV Auger peak.

[1] G. A. Medvedkin *et. al.*, Jpn. J. Appl. Phys.**39**, L949 (2000)

* ishida@wyvern.phys.s.u-tokyo.ac.jp