Electron Spectroscopic Studies of Vapor-Deposited Cobalt Layers on Molybdenum(VI) Oxide Surfaces

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The modification of polycrystalline MoO_3 surfaces by vapor-deposited Co atoms at a substrate temperature of 800 K was studied by means of X-ray photoelectron spectroscopy (XPS). From previous experiments [1] it is known that thin MoO^3 layers react with evaporated Co atoms already at 90 K. At 300 K this process proceeds with a significantly higher reaction rate. The Mo^{6+} 3d signal shows an exponential decay with increasing Co coverage. Simultaneously two new signals are observed in the Mo 3d XP spectra, which are assigned to Mo^{4+} and Mo^{5+}. Cobalt is initially oxidised to Co^{2+} in the surface layer, but with increasing evaporation time the Co0 intensity steadily increases. Annealing of the sample up to 800 K after evaporation results in a small decrease in the Mo4+ concentration and causes a shift of the Mo^{6+} signal towards lower binding energies.

During evaporation at a substrate temperature of 800 K, after an initial increase, a steady state of the Mo^{5+} and Mo^{6+} intensities develops (nominal Co layer thickness ~1 monolayer). Thereafter at constant evaporation rate no significant variations of the concentrations are detected within the escape depth of the photoelectrons. This behavior is attributed to interdiffusion processes in the surface and interface layers. A satisfying fit of the Mo 3d spectra can only be obtained, when an additional Mo^{6+} species is assumed, which is assigned to a cobalt molybdate, in agreement with literature data [2]. The concentration of the Mo^{4+} moiety is negligible under these experimental conditions and the vapor-deposited Co atoms are oxidised quantitatively to Co^{2+}.

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A compact Compton polarimeter utilizing silicon drift detectors

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A compact 90-degree compton polarimeter has been developed and calibrated to be used for energy resolved linear polarization analysis of Parametric X-radiation (PXR) in the energy range from 2 to 20 keV.

The polarimeter employs 4 thermoelectrically cooled silicon drift detectors (Silicon Drift Detector Module SDD 2/5 of KETEK GmbH) viewing a conical beryllium scatterer from azimuths spaced by 45 degrees to measure the modulation of Compton scattering yields. The polarization sensitivity of the device has been calibrated with monochromatized synchrotron radiation of known linear polarization properties. The analyzing power is close to unity in accord with expectations from Monte Carlo simulation results. The orientation of the polarization plane is determined to within a few milliradians. The measured vertical profile of the linear polarization component outside the synchrotron plane agrees with calculations.

The drift detector polarimeter shows substantially better spectroscopic performance and rate capability than a previously described Compton polarimeter employing conventional silicon pin diodes [1]. At a temperature of 260 K and a signal shaping time constant of 500 nsec an electronic noise contribution of 10 electrons (r.m.s.) has been measured. The drift detector polarimeter will be used to analyze PXR polarization properties at large emission angles where unfavourable signal-to-background ratios are to be expected. Energy measurement is the most effective means of background rejection in PXR studies.

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Stereoscopic Photographs of Atoms taken by Spherical-mirror Analyzer*

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Usually stereoscopic photographs of atomic arrangement are produced by computer, but it has never been measured directly. In this study the first "measurement" of stereoscopic photographs of atomic arrangement is reported. This method utilizes a new phenomenon found recently by Daimon et al.[1,2], who observed circular dichroism in photoelectron diffraction patterns from non-chiral and non-magnetic materials. The forward focusing peaks are found to be rotated in the same direction as the spin of the incident circularly polarized light. Their rotation angles around the photon incident axis are well reproduced by a simple formula derived by Daimon et al.[1]. The rotation angle is in proportion to the magnetic quantum number m of the photoelectron, inversely proportional to the distance R between the emitter and a scatterer. The analysis [3] showed that the relation between the distance and the angular shift is the same as the actual view in some condition. Then the photoelectron diffraction pattern obtained by left and right circularly polarized light can be used as stereoscopic photographs.

An example is shown by diffraction patterns of W 4f photoelectrons from W(110)1x1 surface at the kinetic energy of 800 eV. Experiment was performed at BL25SU in SPring-8 [4]. A new display-type spherical-mirror analyzer [5] was used to obtain the patterns. The pattern shows many forward peaks at directions of the crystallographic axes. Their peak positions are rotated from those observed in XPD [7] or their crystallographic axes. Such peak rotations are of the same type as seen for Si(001) [1] and W(110)1x1-O[2]. When we use this pattern as stereo view, <100> and <111> atoms look close and <311> or <211>, and <310> or <210> atoms are far corresponding well with real structure. Hence we conclude that stereo view of atoms are successful.

*Work supported by a Grant-in-Aid for Specially Promoted Research Project from the Ministry of Education, Science and Culture Japan

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Valence, spin-state and neighbour-atom selective XAFS with sub-lifetime resolution

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Selective x-ray absorption fine structure (XAFS) is an important enhancement of the use of XAFS to determine the local geometric, electronic and magnetic structure. Selectivity can be obtained for the valence, the spin-state and the neighbour atom. This opens a wide range of new experiments, for example with valence-selective XAFS the difference in local structure of an element present with two valences can be studied. With neighbour-selective XAFS the local surroundings of a metal at an interface can be separated from the bulk signal, etc [1,2].

The crucial ingredient of selective XAFS and its related techniques (resonant x-ray Raman, etc), is the combination of high-resolution x-ray monochromators for both the incoming and emitted x-rays.A number of recent applications will be discussed:

(1) To show the importance of the removal of the life time broadening, the L1, L2 and L3 edges of Pt metal have been measured. The sub lifetime resolved spectra show close agreement with the empty density-of-states (as calculated using FEFF8). This opens the way to study changes in the density of states due to adsorption. Results will be shown on the study the hydrogen adsorption on supported Pt catalysts.

(2) It is shown that the magnetic linear dichroism effect in x-ray emission is a direct probe of the magnetic moment. With respect to x-ray absorption MCD, emission MLD possesses the advantage that only hard x-rays are involved and no circular polarisation is needed. With the complications related to electron detection, soft x-ray experiments and circular polarisation disappearing, applications include the study of buried magnetic systems in-situ, at high pressure, temperature and magnetic fields [3].

(3) The related technique of resonant x-ray Raman scattering can be used to study the local spin-flip spectral distribution in magnetically ordered 3d transition-metal compounds. It is shown that the scattered x-ray energy and intensity distribution contains the excitation spectrum resulting from a single local spin flip, as well as dd excitations accompanied by local spin flip satellites [4].

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Coherence In Two-electron Transfer In F^{8+}+ Ne Collisions*

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The study of multielectron transitions in atomic collisions provides insight into the fundamental nature of atomic structure and the collisional dynamics by probing interactions that go beyond the independent electron model. In this work, two-electron transfer leading to the formation of autoionizing projectile 2l2l' states, specifically, F^{8+}(1s) + Ne → F^{6+} (1s2l2l'), are considered. The measurements were done at Western Michigan using the tandem Van de Graaff accelerator. Autoionization spectra for collision energies ranging from 0.5 to 1.75 MeV/u (4.5-8.4 a.u.) have been obtained. Strong variations in the relative 1s2l2l' intermediate state populations as a function of collision energy are observed. Based on auxiliary measurements for a He target, we can infer that for a Ne target the two-electron transfer occurs mostly with at least one electron originating from the K shell. This is consistent with a velocity matching argument for capture at high projectile energies. Furthermore, the relative probability for double K-shell capture is expected to increase with projectile velocity. These results are substantiated by the measured spectra, where we observe that the relative contribution of the 1s(2s2p ^{3}P) ^{4}P line, which must formed with at least one electron originating from the L-shell, decreases with energy. Particularly noteworthy is the relatively small 1s(2s2p ^{3}P) ^{2}P- line, for which the captured electrons have their spins aligned, compared to the 1s(2s2p) ^{2}P- intensity. Based on the large ^{4}P intensity (for which the captured electron spins are also aligned), the 1s(2s2p ^{3}P) ^{2}P- intensity would be expected to be greater than the 1s(2s2p ^{1}P) $^2P_+$ intensity, if the transfer of the two electrons involved independent events. Thus, the strong suppression of the $^2P_-$ line suggests that quantum mechanical coherence effects play a significant role in the two-electron transfer process. Since $^2P^+$ and $^2P_-$ are not pure states, but rather involve configuration mixing, it appears that the amplitudes contributing to these states interfere constructively for $^2P^+$ and destructively for ^{2}P-. Support for this conclusion is provided by the fact that the relative contributions of ^{2}P- and $^2P^+$ increase similarly with increasing projectile velocity, while the relative ^{4}P intensity decreases significantly.

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division.

Double-K-Shell Vacancy Production In Li-Like C$^3+$ Ions Colliding With Helium*

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We have measured the formation of double-K-shell vacancies (hollow ions) in collisions of ~0.5-1.7 MeV/u Li-like C^{3+} ions with helium. The focus of this work is to determine the mechanisms responsible for these two-electron transitions. Of particular interest is the role of the electron-electron (*e-e*) interaction, the strength of which decreases relative to the nucleus-electron (*n-e*) interaction with increasing projectile Z. Although separate *n-e* interactions may play the dominant role in double-K-shell vacancy production of the Li-like projectiles, the helium target electrons may also contribute, including threshold effects with increasing projectile velocity. The present measurements are being conducted at Western Michigan University using the tandem Van de Graaff accelerator. The double-K-shell vacancy states that have been observed are $2s^2\ ^1S$, $2s2p\ ^3P$, and $2s2p\ ^1P$. No significant contribution from the 2l3l' configurations was observed. The present work follows from recent results for relativistic highly charged ions colliding with an atomic Li target [1]. Apparently no three-electron double-K-shell vacancy states (i.e., double-K-shell excitation) are observed for C^{3+} ions, a result that is in agreement with the Li target data [1]. At the lower velocities studied here, dipole transitions are not expected to dominate so strongly the excitation processes. Additionally, connections of ion-induced double-K-shell vacancy processes to photo-induced processes are not likely to be as pronounced.

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This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division.

Spin - Polarized Electron Spectroscopy Study of Strained Semiconductor Heterostructures

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Polarized electron transport in strained semiconductor heterostructures was investigated by means of electron photoemission under circularly polarized light excitation. High resolution energy distribution curves (EDC) and a polarization versus energy distribution curves (PEDC) of the electrons, photoemitted from strained GaAs/GaAsP layers are experimentally studied. In the vicinity of the photoexcitation threshold the polarization does not vary across the energy distribution, which means that no depolarization occurs during energy relaxation in the band bending region (BBR). The electron energy distribution is interpreted in terms of the electron energy relaxation in the band tail states of quantum well formed by the BBR.Polarized electron emission from a series of new strained short-period AlInGaAs/AlGaAs superlattices (SL) is investigated as well. The In layer content was chosen to give minimal conduction-band offset with large strain splitting of the valence-band. Simultaneous changing of Al content in both SL layers provides variation of the structure band gap. We demonstrate as well that tuning of the SL to the excitation energy can be achieved without loss of the electron polarization. The polarization of up to 86% was measured at room temperature. The features of the structures studied make them very promising for the sources of polarized electrons for high energy physics and surface physics applications.

*Work supported by the Russian foundation for Basic Research.

Photoelectron Emission Microscopy and Imaging of Ferromagnetic and Antiferromagnetic Domains

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Photoelectron emission microscopy (PEEM) using polarized x rays is a unique tool for the study of ferromagnetic (FM) and antiferromagnetic (AFM) materials. FM materials are studied using x-ray magnetic circular dichroism (XMCD) and AFM materials using x-ray magnetic linear dichroism (XMLD). The elemental specificity of PEEM allows to study individual layers in multilayer structures, and to investigate the coupling between them. Increasingly complex layered structures containing magnetic and antiferromagnetic materials are used in modern magnetic devices, and knowledge of the magnetic properties of the layers and interfaces is essential for the understanding of the properties of these devices. Of particular interest is the effect of exchange biasing at the interface of an AFM and an FM. AFM materials have been difficult to study so far because of a lack of methods with sufficient spatial resolution and surface sensitivity. We have investigated the magnetic and topographic surface structure of several AFM materials, in particular thin singlecrystalline and polycrystalline NiO and LaFeO$_3$ films. We were able to resolve the antiferromagnetic surface structure of those materials, showing antiferromagnetic domains, and antiferromagnetic patterns, correlated to the surface topography. Local NEXAFS spectra yielded information about the antiferromagnetic orientation at the sample surface. The study of an FM Co thin film on top of an AFM LaFeO$_3$ film showed for the first time a direct correlation between AFM and FM domains, and co-linear alignment between the AFM and FM spin orientation.

Double Ionization Satellites In the L$_2,3$-Auger Spectra of the Argon-Like Molecules

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The molecular C-VV (core-valence valence) Auger spectroscopy which studies the transitions from singly core-ionized states into double-ionizes valence states is a principal tool to investigate double-ionized valence states in molecules. The first experiments in this field were performed more than 25 years ago [1,2]. Recently, new interest in C-VV Auger spectroscopy has arisen due to the possibility of obtaining high-resolution Auger spectra [3]. These new experiments made topical the problem of the detailed assignment of molecular Auger spectra and of understanding the mechanisms of their formation.

Normal L$_2,3$-VV and satellites L$_2,3$V-VVV Auger spectra of HCl, H$_2$S, PH$_3$, SiH$_4$ are calculated by the method on one-centre expansion of Roothaan's MO LCAO [4]. Our calculation includes:

- spin-orbital splitting of the initial 2p-level ;
- multiplet splitting and final-state configuration mixing;
- contributions from ligands AO in transition amplitudes;
- obtaining of the Auger electron wavefunction with taking ligands potential into account.

Probabilities of double ionization upon creation of initial L-vacancies are calculated in sudden limit. Relative probabilities of the satellites spectra are about 10%. Inclusion of double-ionization satellites makes the agreement of the theoretical and experimental spectral profiles better. In some cases inclusion of these satellites allows one to assign certain features in molecular Auger spectra.

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Two-Photon Excitation/Ionization of Inner Shell of Atoms and Ions

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Cross sections of two- and three-photons absorption by many-electron atoms' outer shells are calculated in refs [1-3]. The analogous investigations in the region of absorption thresholds in the X-ray range of photon energy are absent now. The aim of this work is to calculate the cross sections of two-photon absorption by inner shells of atoms [4,5] and ions with inclusion of the relaxation effects.

In this work we present the results of theoretical investigation of the absolute values and the shape of the two-photon one-electron excitation/ionization cross sections of both 1s-shell of neon atom (and its ion Ne$^6+$) and the 1s-, 2s- shells of argon atom (and its ions Ar$^6+$, Ar$^8+$). The results are obtained taking into account the effects of relaxation of the atomic residue in the field of the creating vacancies and the effect of vacancy stabilization (for the ions). The results of calculation have the character of prediction. The fulfilled investigation shows that the process of two-photon excitation/ionization of the inner shells of both atoms and ions have essentially the many-electron character. It follows to note that the inner shells expose itself already at the photon energies significantly less than the ionization potentials of these shells. This theoretical prediction can be experimentally verified using the existing lasers.

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Orientation of the Ar 2p$^-1$, Kr 3d$^-1$ and Xe 4d$^-1$ hole states*

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The photoionization process can be described by transition amplitudes and relative phase shifts of the outgoing electron waves. The number of parameters needed is model dependent. However, even for the simplest model - the LS-coupling - the determination of partial cross section and angular distribution values is not sufficient to derive such amplitudes and phase shifts. In many cases, additional information can be retrieved from the analysis of the alignment or orientation of the remaining ion [1,2]. While alignment can be created by any kind of particle or photon impact, orientation requires excitation by polarized particles or circularly polarized photons. We have performed such an experiment by carrying out spin polarization measurements of Auger lines following the Ar 2p, Kr 3d and Xe 4d photoionization. These measurements were carried out at the new elliptical polarization undulator (EPU) beamline of the Advanced Light Source (ALS) using the 1st harmonic of the undulator without a monochromator. Using the ^{1}S$_0$ Auger lines we could derive the orientation parameter A$_10$ of the Ar 2p$^-1$, Kr 3d$^-1$ and Xe 4d$^-1$ hole states over a broad photon energy range. The results will be compared to various theoretical calculations and complementory measurements of the alignment or the spin polarization of the photolines.

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*Work supported by the Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences Division.

Angular distribution of ligand-field split components of iodine 4d photoemission in HI molecule*

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Angular distribution of core-level iodine 4d photoelectrons from the HI molecule was measured using synchrotron radiation in the 80-150 eV photon energy range. The anisotropy parameters of all five ligand field split components ($\sigma_{1/2}$, $\pi_{1/2,\ 3/2}$, and $\delta_{3/2,5/2}$) of the iodine 4d photoelectron spectrum were determined and found to be equal within experimental uncertainties at all photon energies. A comparison of the photoelectron angular distribution of HI and Xe shows that the molecular 4d photonioization is well described by an atomic model. From high-resolution spectra, the lifetime widths of the I 4d hole states were determined.

*Work supported by the Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences Division.

Electron ion Velocity Vector Correlation study of Dissociative Photoionization of O_2 of Dissociative Photoionization of O_2*

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The Velocity Vector Correlation method is a new tool for the investigation of (DPI) dissociative photoionisation. DPI processes are characterised by three vectors (VA+,Ve- and P),the ion and electron velocities and the light polarisation respectively. AB + hn --> AB** --> A+ + B+ e- . Measurement of the correlation between VA+,Ve- for each phtoionisation event in a coincidence experiment provides:
i: the dissociation channel Ed = E (A+) + E (B) = hn - Ek (A++B) - Ek (e-) (1)
ii: the angular distribution of the fragment ions and electrons in the laboratory frame
iii: the angular distribution of the electrons in the molecular frame (spatially oriented molecules)

We designed a double (TOF) time of flight velocity spectrometer with = 4p steradians acceptance angle for both charged particles that combines time and position sensitive detection and imaging techniques. We report the DPI study of O2 in the region 22 - 24.4 eV. Oxygen molecules in a pure or He seeded beam were ionised using pulsed, linearly polarised and dispersed synchrotron radiation from Super ACO at Orsay. The experimental set-up was briefly described in previous reports1,2. Electrons and ions produced at the centre of the light and molecular beam interaction region are accelerated in opposite direction by a DC field. From the positions and TOF one derives the three components Vxe, Vye, Vze and Vxi, Vyi, Vzi of the VA+,Ve- velocities. Any combination of two variables can be represented in a two dimensional histogram for visual and quantitative analysis.

The histogram presented in figure 1 represents the correlation between electron and fragment ion energies after excitation of O$_2$ at 23.15 eV. The vertical axis (Ecmi_e) shows the value of Ed as calculated using equation 1 as a function of (Ecmi) the O+ kinetic energy. Note that in the limit of infinite resolution the data points would accumulate along horizontal lines. The dominant process is observed in the first O$^+$(^{4}S) + O(^{3}P) dissociation channel at 18.733 while two minor ones are observed in the second O$^+$(^{4}S) + O(^{1}D) and third O$^+$(^{2}D) + O(^{3}P) dissociation channels at 20.70 and 22.06 eV respectively. The excitation energy falls in a Franck-Condon gap region between the B ^{2}S$_g$$^-$ and III^{2}P$_u$ states of O$_2$$^+$ where no state of the molecular ion can be directly excited(3), hence DPI processes may result either from excitation of B ^{2}S$_g$$^-$ and b^{4}S$_g$$^-$ states of O$_2$$^+$ and / or from autoionisation of dissociative resonance states. Excitation of the 18.733 eV channel is mainly explained by the formation of the B state. The peaks observed at Ecmi = 0.14 and 0.5 eV in the 22.06 channel result from complete dissociation of the Rydbergs with n* = 3 and 4 into O(^{2}P, nd") + O(^{3}P) and autoionisation of the excited atoms to O$^+$(^{2}D).

The O$^+$ angular distribution in the laboratory frame was measured and illustrated the perpendicular character of the O$_2$^{3}S$_g$$^-$ (n = 3, 4) ^{3}P$_u$ transitions which in turn confirmed the assignment given in previous investigations(3,4). The electron angular distribution in the frame of the dissociating molecule was also measured for all orientation of the molecular axis. It showed similar anisotropies for n=3 and n=4. At this level of the analysis the latter distribution confirms the interpretation of previous results on O$^+$ angular distribution correlated with electrons emitted in a fixed direction(4).

In conclusion the electron ion velocity correlation method is shown to resolve the various processes involved in dissociative photoionisation of oxygen molecule. Autoionisation of valence repulsive Rydberg states are seen to contribute to the production of O^+ fragments in several dissociation channels. Complete dissociation prior to autoionisation leads to atomic autoionisation while autoionisation en route to dissociation results in the population of vibrational continua of bound electronic states of the ion. Angular distributions of the ions in the laboratory frame and electrons in the molecular frame that are obtained with this method are unique tools to unravel the symmetries and relative contributions of degenerate electronic and nuclear continua.

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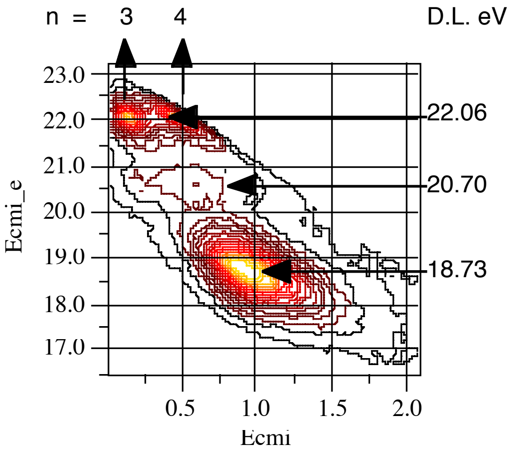
ICESS 2000 Abstract Guyon figure 1



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Electronic Structure Contributions to Redox Potentials in High Spin Iron Species.

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Core and valence photoelectron spectroscopy are used to define the electronic structure contributions to redox potentials. We have used variable energy PES to study $[FeCl_4]^{1-/2-}$, $[FeS_4]^{5-/6-}$ and $[Fe(SR)_4]^{1-/2-}$ to estimate the relative contributions of the effective nuclear charge (Z_{eff}), the energy of the redox active HOMO and electronic relaxation to redox thermodynamics. $[FeCl_4]^{2-}$ shows considerable electronic relaxation on oxidation and as a result of spin polarization the ferric species exhibits an inverted bonding scheme. The 1.0V shift in the redox potential between $[FeCl_4]^{2-}$ and $[Fe(SR)_4]^{2-}$ is attributed to the greater ability of the thiolate ligand to stabilize the oxidized state due to the covalent interaction with the metal center and the presence of low lying excited states. These studies have been further extended to $[FeCl_6]^{3-/4-}$ to address the coordination number effects on redox potentials. Density functional calculations are correlated to experimental data to provide additional insight about contributions to redox.

Spin polarization in the resonant Auger decay of argon*

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The dynamics of the photoionization and Auger decay processes can be fully described by the dipole and Coulomb transition matrix elements, respectively. A complete set of matrix elements, amplitudes and phase shifts, enables the prediction of all parameters of the emission process, such as the angular distribution and spin polarization of the electrons. For this reason, big advancements were made in complete photoionization experiments in recent years [1,2]. In contrast, there have been only very few studies of the Auger decay process beyond Auger intensities and angular distributions [3], although Auger spectroscopy is an important field of research in gas-phase, solid state and surface physics.

We have made the first measurement of spin polarization of resonant Auger electrons emitted from the decay of the Ar 2p$^-1$->4s and 2p$^-1$->3d excited states. We used monochromatized, circularly and linearly polarized light of 244 eV photon energy from the new elliptical polarization undulator (EPU) beamline of the Advanced Light Source (ALS) to carry out the experiment. Some of the Auger lines show a high degree of polarization, which will possibly enable the determination of Coulomb matrix elements.

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*Work supported by the Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences Division.

Effects of Ca-doping on Local Structure in RBa2Cu3O7-£_ Systems (R = Y, Gd, and Nd)

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Ca-doping generates excessive holes and suppresses the superconducting transition temperature Tc of RBa2Cu3O7-£_(R123) due to the over doping effect. Relatively, Tc and the normal state resistivity of R123 systems also dependent on the ion size of rare-earth (R). In order to study the effects on local structure around CuO2 plane due to Ca-doping in RBa2Cu3O7-£_ systems, we have performed extended x-ray absorption fine structure (EXAFS) measurement on two series of R1-xCaxBa2Cu3O7-£_ samples (for R=Gd: x=0, 0.1 and 0.2; for x=0.1, R=Y, Gd and Nd) at room temperature. Our results show that in the Gd system, Cu-O bond distance and static disorder, as indicated by Debye-Waller factor, increase with Ca concentration. For samples with different rare-earths but same Ca content (x=0.1), we found the static disorder of the surrounding atoms increases with the radius of the R3+ ion. No significant changes in the coordination number of O surrounding Cu were observed. We conclude that the decrease of superconducting temperature due to Ca-doping and the increase of the normal state resistivity with R3+ ion size are both related to the increased static disorder of the lattice.

Time-resolved photoemission from image-potential states

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Electrons attracted by the image force to a metal surface are loosely bound and form a Rydberg-like series of states converging towards the vacuum level. Energies and lineshapes of these image-potential states are studied by two-photon photoelectron spectroscopy. The use of Ti:sapphire lasers as light sources has raised the count rates by several orders of magnitude and added the possibility to study the lifetime in the femtosecond range.

Coherent excitation of several higher image-potential states of the Rydberg-like series leads to the observation of quantum beats in the time domain. The decay of the beat pattern can be controlled independently from the lifetime by selection of suitable adsorbates. The same information can be obtained for the lower image-potential states from a careful analysis of linewidth and lifetime measurements. The dependence of the various decay mechanisms on quantum number and adsorbate will be discussed. The model system of image-potential states can be studied extremely well in present experiments and the results contribute to
the understanding of photochemical processes and hot-electron dynamics at surfaces.

SPLEED under the Existence of s-f Interaction

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Spin polarization of electrons scattered on the surface of a magnetic material, in which spins are mainly caused from the presence of unshelled f electrons, is discussed and examined on the basis of the Anderson-Newns Model. When analyzing the above system, we assume that [1] the kinetic energy of incident electrons is as low as Fermi level(¢≈ the order of several eV) [2] the effect of LS coupling can be negligible and [3] absorption of incident electrons on surface can be also negligible. In such an case as above , it is supposed that because of very low kinetic energy ,incident electrons can be strongly influenced by the presence of spins on surface; thus we can not reduce such a system to one body problem in which the influence of surface including spins could be possibly expressed in the form of one body potential. In stead, many body problem caused from exchange of incident electrons on surface appears(s-f interaction); accordingly we evaluate the effective Hamiltonian and calculate transition probability, using Fermi rule and perturbation method. From the analysis on polarization of spin in Curie-paramagnetic material, though the difference between the number of electrons with ¡©up or down spin increases with external field, only a little difference is observed even when a large external field is applied. In ferromagnetic materials in the temperature range of T ¢≈Tc, scattering polarization asymmetry seems to be proportional to the¡¡surface magnetization.

Spectromicroscopic Investigation of Nonlinear Photoemission and Hot Spots on Surfaces by Means of PEEM Combined with High Power Laser Radiation

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The interaction of high intensity pulsed laser radiation with surfaces results in nonlinear optical effects that are responsible for emission of electrons even if the photon energies are below the work function threshold of a solid. In the present study, photoelectrons have been excited by means of high-power femtosecond laser pulses with a photon energy below the work function threshold. The spatial distribution of the photoemission yield was imaged utilizing photoemission electron microscopy (PEEM). The second order electron yield of the metallic as well as organic films (Lead and Permalloy) adsorbed on silicon depends strongly on the sample topography and the polarization of the photons.

A strong spatial variation of the nonlinear photo-yield was observed in electron emission from all thin films adsorbed on silicon. Centers of enhanced high-order yield, so called 'hot spots', were observed on the surface of various samples. These hot spots were preferentially excited with s-polarized light. This observation is in contrast to other investigations of nonlinear phenomena from rough surfaces.

The order of nonlinear processes in photoemission was visualized introducing logarithmic scaled images. A mapping of the order of the nonlinear effects in photoemission from Pentacene covered silicon exhibited a third order process at rough sample areas being preferentially excited with s-polarized laser radiation. In contrast to the case of metallic films, this effect cannot be attributed to localized plasmon modes. Doping of the Pentacene layers lead to a decrease of the order of the nonlinear photo yield. The decrease was found to be stronger on Pentacene covered areas compared to bare parts of the sample.

Support by the NSC of Taiwan (Contr.No.: 89-2811-M-001-0002) is gratefully acknowledged.

The Temperature Dependence of the Circular Dichroism in Angular Resolved Photoemission from Rare Earth Surfaces: Gd(0001)

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Circular dichroism can be observed in angular resolved photoemission from magnetized as well as paramagnetic materials. That means it is not restricted to investigate magnetized samples at temperatures below the Curie temperature. In a first approximation the circular dichroism is a phenomenon observed from oriented atoms. In photoemission from solid surfaces additional features will appear that have to be taken into account.

In the present study the circular dichroism in angular photoemission is investigated theoretically by expanding the free atom methods in a three-step photoemission model. The calculations are performed for the 4l (l=s,p,d,f) states of ferro- and paramagnetic Gd(0001) surfaces. The scattering of the photoelectrons is treated relativistic using full symmetry potentials. The temperature enters the calculations in two ways namely it changes the initial and final states. This is respected by means of simple models for a first approximation. The temperature influences the scattering of the photoelectrons due to lattice vibrations, what is respected by a Debye-Waller model. The temperature dependence of the atomic orientation is respected using molecular field theory. The saturation magnetization in dependence on the temperature influences not only the orientation of the initial state but also the exchange part of the scattering amplitudes. These simple models already show that the temperature dependence of the magnetic circular dichroism is not simply proportional to the saturation magnetization of the sample. In particular close to the Curie temperature one finds that the gradient of the dichroism is stronger than that of the saturation magnetization.

Support by the NSC of Taiwan (Contr.No.: 89-2811-M-001-0002) is gratefully acknowledged.

Photoelectron Holography using Circularly Polarized Light

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Circular dichroism in the angular distribution of photoelectrons (CDAD) is not only observed from aligned or oriented initial states, but also as a consequence of the scattering of photoelectrons at the surrounding atoms in a solid or an adsorbate. Meanwhile, CDAD was measured in photoemission from several statistically isotropic distributed initial states. The results can be explained if photoelectron-diffraction is taken properly into.

The CDAD from a core-level can be described by a simple model using single scattering plane wave approximation [1]. The analytically derived CDAD can be interpreted to be an integral transformation of the product of the angular momentum of the emitted electron and the Fourier-transformed scattering potential of the surrounding atoms. Therefore, the CDAD pattern from core levels can be looked at as a photoelectron hologram. The real space pattern can be reconstructed by the inverse integral transformation of the CDAD pattern. Like in CDAD from aligned or oriented states one observes intensity only from mixed products of the final state partial waves, that are here the scattering interference terms carrying the full phase-information. Because of the nature of the CDAD there is no need to make any assumptions about background-substraction like in holography from conventional XPD [2]. Due to the angular momentum transformation the anisotropic nature of photoelectrons is accounted automatically. It will be shown for the simple case of emission from s-states, that a CDAD pattern, taken at only one kinetic energy, can be used for a three-dimensional reconstruction of the real space with a reasonable resolution if the full half-space above the sample is respected. Multi-energy scans using only parts of the half-space will be suitable for experiments, due to the restricted angular range available.

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X-ray-excited optical luminescence of erbium-doped semiconductor: Site-selective x-ray absorption spectroscopy of an optically active atom

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X-ray-excited optical luminescence (XEOL) of erbium-doped silicon (Si:Er) thin films is observed for site-selective x-ray absorption spectroscopy (XAS) of optically active Er atoms. Although conventional XAS evaluates the x-ray absorption of the entire Er, XAS using XEOL provides structural and electronic information of only the optically active Er. XAS using XEOL from a mixture of semiconductors [1] or rare-earth powders [2] has already been demonstrated. However, since luminescence from the appropriate optical centers excited by the x-ray absorption of the bulk atom is observed in these studies, site-selectivity at the atomic level has never been achieved.

The experiments were performed at SPring-8 BL29XU RIKEN beamline, in Hyogo prefecture, Japan. The Si:Er thin film was deposited by a laser ablation technique. The Ge p-i-n photodiode with an infrared (IR) monochromator was used to detect XEOL of Er intra-4f transition.

At a low sample temperature of 20 K, IR luminescence related to Er was observed under x-ray irradiation with photon energy between 8.3 and 8.5 keV, indicating that the 4f electron is excited by x-rays even below the Er LIII-edge (8.36 keV). This result suggests that the x-ray beam produces the electron-hole (e-h) pair in Si bulk, and a subsequent recombination excites the 4f electron of Er. This undesirable luminescence independent of the inner-shell excitation increases the background level and disturbs XEOL signal detection. In effect, the x-ray absorption spectrum does not observed in the x-ray photon energy dependence of the luminescence intensity at this temperature. On the other hand, the edge-jump and absorption peaks at the Er LIII-edge are obtained at 300 K. This result can be explained as follows. Since the recombination energy of the e-h pair is mainly used for phonon excitation without the optical transition in the high-temperature region, the background luminescence due to the bulk absorption is suppressed. The spectrum at 300 K originates from the inner-shell excitation and relaxation of only the optically active Er atom, resulting in the fact that site-selectivity at an atomic level is realized.

The energy width of a 2p-5d resonant absorption peak observed by XEOL is broader than that measured by the conventional method, indicating a dispersive 5d electronic state in the optically active Er. The optically inactive Er has a concentrated 5d state caused by a higher order symmetry [3]. The conventional XAS observes the average state of the optically active and inactive Er atoms in the thin film, so that a more concentrated 5d state than the actual one is equivalently obtained.

Hydrogen Adsorption on a HfC(111) Surface: Angle-Resolved Photoemission Study

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Angle-resolved photoemission spectroscopy (ARPES) utilizing synchrotron radiation has been applied to study the adsorption state of hydrogen on a HfC(111) surface. It is found that hydrogen adsorbs dissociatively on the HfC(111) surface at room temperature forming a (1x1) overlayer at saturation coverage. A H 1s-induced split-off state (bonding state) is observed at 7.2 eV in normal emission spectra at saturation coverage. The two-dimensional band structure of the H 1s-induced state is investigated by off-normal-emission measurements. The band width of the state is estimated to be 1.0 - 1.2 eV, which is comparable to those obtained for H/TiC(111) [1] and H/ZrC(111) [2] systems. In addition to the H 1s-induced state, another H-induced state is found in the off-normal-emission spectra just below the Fermi level. The state is ascribed to the extrinsic surface state arising from the H-induced modification of surface electronic states, as has been proposed in a theoretical study [3].

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Spin-polarization and dichroism in electron spectroscopy from atoms, molecules, and adsorbates

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Very resently measured circular dichroism data in the angular distribution of photoelectrons (CDAD) of free unoriented campher and bromocampher chiral molecules are presented for the first time. New results of the angular distribution of the spin polarization of Augerelectrons from Kr and Xe atoms obtained at the new helical undulator UE 56/1 of BESSY II enabled to determine the dynamical spin parameters for Augeremission for the first time. The talk additionally reviews the spin polarizations of photo- and Auger-electrons of free as well as adsorbed Iodine molecules and compares the data with the corresponding results of the isoelectronic Xenon atom. The data are discussed towards the goal of a quantummechanically complete characterization of the Photo- and of the Auger-process. Finally the influence of molecular rotation on to the photoelectron spin polarization is also discussed.

Compton photon-electron coincidence spectroscopy studies of 3D-electron momentum densities in solids

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If in deep inelastic X-ray scattering (i.e. Compton scattering) the momenta of the scattered photon and its recoil electron are measured simultaneously one can reconstruct the momentum of the electron in its initial state in a unique way. At the same time the triple differential cross section for such a coincidence experiment factorizes into an essentially constant cross section part and the electron momentum density (EMD) of the electron. We have applied this technique to solids. The overwhelming part of experimental techniques for the investigation of the electronic structure of solids is concerned with the study of energy dispersion or density of states (UPS, EELS, XAS, IXS). In contrast, only a few methods exist which measure directly wave function related quantities like EMD's. We mention that the well known positron annihilation technique does not measure the EMD but the electron-positron pair density which is different from the EMD.

Using the intense x-ray radiation of 3d-generation synchroton radiation sources (ESRF, PETRA), we have measured the 3D-EMD of graphite, fullerenes, Al and Cu/Ni alloys and compare them with nowadays band structure calculations (FP-LMTO, MAPW, KKR-CPA). The experiment is able to distinguish between these theories.

Ion desorption induced by the shake-up excitation from H_2O/Si(100)

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The electron-ion coincidence spectroscopy is a recently developed tool for investigating ion desorption from solid surfaces induced by the core-level excitation. In this study, we apply this technique to H^+desorption from water chemisorbed Si(100) surface induced by the photoexcitation of the O1s level. When the H_2O/Si(100) surface is irradiated by a photon of 680eV, the desorption of H^+ is observed in coincidence with a photoelectron emission of not only the O-1s main peak but also of its shake-up/off satellites, the excitation of the valence levels taking place simultaneously. The analysis of the spectra shows that more than 2/3 of H^+ desorb as a result of the shake-up/off excitation. According to previous results using Auger-electron ion coincidence spectroscopy [1], it has been found that the shake-up/off process to occur simultaneously with the Auger decay of the O1s hole is predominantly responsible to the H^+ desorption. These results indicate that most of the H^+desorption from the H_2O/Si(100) irradiated by soft-X ray is stimulated by multielectron excitation/decay which induces a multi-hole($n>2$) creation, rather than normal Auger decay resulting in the two holes.

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Measurement of Silicon Dioxide Film Thicknesses by XPS

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It is now customary for the effects of elastic-electron scattering to be ignored in measurements of overlayer thicknesses by XPS. It is known, however, that elastic scattering can cause the effective attenuation length (EAL), needed for the thickness measurement [1], to be appreciably different from the corresponding inelastic mean free path [2]. We have investigated the effects of elastic-electron scattering in measurements of the thicknesses of SiO_2 films on Si from XPS measurements with Al and Mg Kα x rays. Calculations have been made of substrate and oxide Si 2p photoelectron currents for different oxide thicknesses and emission angles using an algorithm based on the transport approximation [3]. This algorithm accounts for the occurrence of elastic scattering along electron trajectories in the solid. It was found that the average EAL, determined from the substrate currents with and without an oxide overlayer of a certain thickness, varied weakly with oxide thickness and emission angle for a restricted range of emission angles. For emission angles greater than about 60°, corrections need to be made to this average EAL in order to determine the oxide thickness. These corrections will be described.

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NIST Databases for Surface Analysis by AES and XPS

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NIST currently offers three databases for surface analysis by AES and XPS [1]:
- X-Ray Photoelectron Spectroscopy Database (SRD 20)
- Electron Elastic-Scattering Cross-Section Database (SRD 64)
- Electron Inelastic-Mean-Free-Path Database (SRD 71)

New versions of these databases are being released in 2000, and the features of these new versions will be described.

Version 3.0 of SRD 20 will be available for on-line access through the internet and will be free. It contains a substantial amount of new data and, for the new data, additional information about the specimen material, measurement conditions, and data-analysis procedure for each measurement. The internet version features redesigned screens to facilitate user access, user searches, and user convenience. This database can be used to identify unknown spectral lines, retrieve data for selected elements, retrieve data for selected compounds, display Wagner plots, and retrieve data by scientific citation. Work is ongoing to provide additional evaluated data for this database.

Version 2.0 of SRD 64 was released in April, 2000. This database provides differential and total elastic-scattering cross sections for elements with atomic numbers from 1 to 96 and for electron energies between 50 and 20,000 eV. These cross sections are needed for simulations of signal-electron transport in XPS and AES (and for other applications involving electron transport). The database also contains transport cross sections (needed for corrections of elastic-scattering effects in AES and XPS) and phase shifts.

Version 1.1 of SRD 71 provides calculated and measured electron inelastic mean free paths (IMFPs) for elements, inorganic compounds, and organic compounds. If no calculated or measured IMFPs are available for a material of interest, values can be estimated from two predictive formulae. IMFPs are needed for quantitative analyses by AES and XPS (corrections for matrix effects), determination of effective attenuation lengths (measurement of film thicknesses), determination of mean escape depths (average depths of analysis), and for simulations of the transport of signal electrons.

*In collaboration with A. Y. Lee, D. M. Blakeslee, J. R. Rumble, Jr., A. Naumkin, A. Kraut-Vass, and A. Jablonski
1. Further information can be obtained from: http://www.nist.gov/srd.

Vibronic Structure in the Carbon 1s Photoelectron Spectra of HCCH and DCCD

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The carbon 1s photoelectron spectra for HCCH and DCCD have been measured at a photon energy of 330 eV and an instrumental resolution about half the natural line width. The vibrational structure in the spectra has been analyzed in terms of a model in which the parameters are the force constants for CC and CH stretching in the core-ionized molecules and the changes in bond-length between the core-ionized and neutral molecules. Within this model, four different approaches to core-hole localization have been considered. Treating the core hole as completely localized, with the molecular motion following the diabatic energy surfaces, does not describe the data correctly. Treating the core hole as completely delocalized, with the molecular motion following the adiabatic surfaces, gives a good fit to the spectra but leads to zero-point energies that are completely unreasonable. Two fits that take into account vibronic coupling between the vibrational manifolds of the ungerade and gerade electronic states of the ions give good agreement with the data and lead to reasonable molecular parameters. Ab initio calculations of the molecular properties of the core-ionized molecule give results that are in good agreement with those obtained from the better of these two fits. The natural line width for the carbon 1s hole, related to the lifetime, is 106±2 meV, significantly higher than for methane (95±2 meV). This result is not in accord with predictions based on a one-center model of Auger decay, but is qualitatively in agreement with the prediction of a multicenter model.

On the Angular Distributions of Electrons Photoemitted from Fixed-in-Space and Randomly Oriented Molecules

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New theoretical expressions are devised from a dynamical perspective for photoionization cross sections differential in electron ejection angles for both fixed-in-space and randomly oriented molecules, and comparisons made with concomitant dipole and nondipole anisotropy factor measurements. The new expressions are obtained in closed forms in terms of body-frame transition moments and related normalized angular-distribution amplitudes which can be calculated employing interaction-prepared states without reference to specific scattering boundary conditions. The leading (dipole) anisotropy factor is similar in form to the familiar Bethe-Cooper-Zare expression for atomic photoemission anisotropies, to which it reduces in appropriate limits. The formalism is employed to relate measured dipole photoemission anisotropy factors to corresponding absorption anisotropies and to the angular distributions of K-shell electrons photoejected from fixed-in-space nitrogen molecules. Measurements of the lowest-order (dipole-quadrupole) retardation terms in nitrogen reveal large deviations from the dipole distributions below 1 keV incident photon energy. These strictly molecular phenomena are accounted for on basis of the new development by the energy variations of the relevant transition moments and angular-emission amplitudes.

Temperature-dependent metal-insulator transition in d- and f-electron systems studied by high-resolution photoemission spectroscopy

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We have observed temperature-dependent metal-insulator transitions (MIT) in Y$_{1-x}$Ca$_x$TiO$_3$ (x~0.4)[1] and a Kondo semiconductor Ce$_3$Bi$_4$Pt$_3$[2] by high-resolution photoemission spectroscopy. Ti 3d and Ce 4f states are dominant near the Fermi level and play important roles in the MIT. We have recognized coherent and incoherent parts in Ti 3d and Ce 4f photoemission spectra. Electron correlation and hybridization effects are important for the temperature-dependent MIT. In the present paper, we discuss the MIT of these compounds from the viewpoint of the temperature-dependent spectral weight redistribution between coherent and incoherent parts around the transition temperature. Small spectral intensity appears at E$_F$ below ~150 K in Y$_{0.61}$Ca$_{0.39}$TiO$_3$. The insulator-to-metal transition is accompanied by the reduction of the relative spectral weight of the incoherent part to that of the coherent part with decreasing temperature. Since hysteresis effect was found in electrical and magnetic measurements, temperature-dependent lattice distortion or bandwidth (W) modulation should contribute to the MIT. Although nominal carrier density of Ti 3d state is less than 1, the MIT can be described from the viewpoint of the Mott transition determined by temperature-dependent U/W (U: d-d Coulomb repulsion). On the other hand, rapid reduction of spectral intensity has been observed for the binding energy range of 0(=E$_F$)-10 meV in Ce$_3$Bi$_4$Pt$_3$ below ~110 K (<T$_K$, Kondo temperature). From the core-level x-ray photoemission studies, f^1 final state is dominant, which is responsible for the Kondo interaction. The relative spectral intensities of satellite structures (f^0 and f^2 final states) to the f^1 state, however, increase as temperature decreases, indicating hybridization effects become important with decreasing temperature. Below a characteristic temperature (~110 K), coherence among "Kondo singlet " develops through hybridization leading to the energy gap formation in the Kondo Lattice.

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Vibrational structure and partial Auger rates of the N 1s core-excited states in nitric oxide

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Resonant excitation of core electrons in open-shell molecules gives rise to several electronic states of different symmetry. In the NO molecule, photoexcitation of the N 1s electrons to the partially occupied valence orbital creates three bands in the absorption spectrum, with strongly overlapping vibrational progressions[1]. Photon-energy-selective resonant Auger spectroscopy provides a tool to study in detail the core-excitation and decay processes and the various excited and ionic states involved. The Auger decay spectra of the core-excited states were measured with vibrational resolution in both photon energy of the VUV-excitation (resolving intermediate excited states) and electron energy (resolving final ionic states). Auger electron spectroscopy was performed at the Advanced Light Source using a hemisherical electron analyzer (Scienta SES-200).

The experimental results are compared with ab initio calculations of the photoabsorption and Auger decay spectra[2]. The Auger decay to the lowest-energy ionic state, being well separated in the electron spectrum, allows to test the accuracy of the calculated potential energy curves by comparing the measured and theoretical vibrational structures. A very good general agreement is observed.The theoretical Auger electron spectra were regenerated according to our experimental conditions. The structure of the simulated spectra resembles the measured spectra closely at all photon energies. For a more quantitative analysis, partial Auger decay rates were determined from the experiment and compared with calculations. They are in good overall agreement, although the experimental and theoretical values differ up to 1.5 times for some ionic states. Some of these discrepancies can be due to unaccounted interference effects.

The high-resolution measurements provide a stringent test for theory at the level of individual electronic and vibrational transitions. Our comparison shows that advanced ab initio calculations can describe the core-excitation and Auger decay processes in open-shell molecules such as NO with high accuracy.

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High Resolution Si 2p Core-Level Spectroscopy for Molecular Adsorption on Si(100)c(4x2) surfaces: The Interface Bonding and Charge Transfer between the Molecule and Si Substrate

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THE IIn recent years, there has been a great deal of interest in molecule-silicon systems, concerning the application to the molecular scale devices. Especially, for alkene/Si(100) systems, the pai bond of alkene interacts with dangling bonds of Si dimer, producing the ordered, anisotropic organic films on Si(100)[1,2], therefore, many extensive studies have been done. However, the nature of the interface bonding in covalently attached molecule-silicon surface systems have been unknown. High resolution core-level spectroscopy provides crucial information about the interface bondings and the charge transfer between molecule and substrate. In the present study, we have investigated the interface bonding and charge transfer between molecule and silicon substrate for the alkene/Si(100) systems by means of high resolution core-level spectroscopy.

The experiments were performed using a BL-16B with an undulator radiation source of Photon Factory at High Energy Accelerator Research Organization in Tsukuba, Japan. In the experiments, the total energy resolution was estimated to be below 80 meV at the photon energy of 130 eV, and the photoelectron spectra were measured at ~ 140 K for clean Si(100)c(4x2) surface, and chemisorption layer on Si(100)c(4x2).

After adsorption of ethylene (cyclopentene) molecules, the peaks corresponding to the up and down dimers completely disappeared, and the new peak observed in ~0.28 (0.32) eV related to the bulk Si peak appeared. The new peaks are assigned to the di-sigma Si-C bonds, considering that the C atom is more electronegative than the Si atom and the area intensity of the Si-C peak is almost the same as the sum intensity of the up and down dimer peaks. Furthermore, it is found from high resolution core level spectroscopy that the charge transfer depends strongly on the molecules.

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A high-energy (e,2e) spectrometer for the measurement of spectral functions

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In an (e,2e) experiment an incoming electron scatters from a target electron, transfering a large fraction of its energy and momentum to this electron, and both scattered and ejected electrons are detected in coincidence. At high energies the interpretation of the (e,2e) measurements becomes very simple. The binding energy E of the ejected electron is equal to the difference in kinetic energy of the incoming electron and the sum of the energies of the outgoing electrons. The recoil momentum p of the target is the difference of the incoming electron momentum and the sum of momenta of the outgoing electrons. The measured intensity I(E,p) is directly proportional to the spectral function of the target [1]. Thus (e,2e) spectroscopy is a high-energy electron spectroscopy that resolves both the binding energy and momentum.

The new ANU spectrometer uses an incoming energy of 50 keV and detects two outgoing electrons with an energy near 25 keV in a transmission geometry. At these energies it is possible to measure targets not thicker than the mean free path for elastic and inelastic scattering. Thus multiple scattering (plasmon creation and/or elastic deflections) probabilities are manageably small and can be corrected for. In spite of the small (e,2e) cross section at these high energies we can, using multiple-parameter detection techniques, measure a set of valence band spectra in a day.

We present the experimental data and the Green's function cumulant expansion calculations of the spectral function for both graphite and aluminum. In order to describe the experiment correctly the theory should not only predict the right dispersion, but also the right intensity, life-time broadening and intrinsic satellite structures. For graphite the theory predicts a strong asymmetry and large width of the quasi-particle peak near the bottom of the valence band. This is confirmed by the experiment. For aluminum the experimental results are not reproduced by either a many-body jellium, or an LMTO-DFT type calculation, but can be described if both electron-electron interaction and the effect of the lattice is taken into account within the cumulant expansion for the Green's function.

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Valence Band Electronic Structures of Pauli Paramagnetic Cr and Ni Pnictides

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A resonance photoemission (RPES), angle resolved ultra-violet photoemission (ARUPS) as well as an inverse photoemission (IPES) (hν =9.4eV) spectroscopies were performed for NiAs and CrP to study their electronic states related to the magnetism and the structural phase transition. The RPES measurement was performed using the synchrotron radiation at BL-7 of HiSOR, Hiroshima Synchrotron Radiation Center (HSRC). The valence band resonance photoemission and Ni 2p XPS spectra of NiAs show the satellite structures accompanied by the main features. It is evaluated that the large energy separation between the main and satellite structures are mainly caused by the strong hybridization effect between Ni 3d and As 4p states. The angle resolved photoemission experiment was done for single crystalline CrP(100) at the BL-18A of Photon Factory, KEK. The experimentally obtained band structures especially for P 3p bands being spread in the energy range of 3-7eV show the remarkable dispersions on the Γ (X)-Y(S) and Γ (X)-Z(U) planes in the orthorhombic Brilloin zone, which are consistent with the result of the band calculation.

Soft X-ray Magnetic Circular Dichroism Study of The Ferromagnetic Spinel-Type Cr Chalcogenides

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We have observed magnetic circular dichroism (MCD) in the soft X-ray absorption spectra of the semiconducting ferromagnet CdCr$_{2}$Se$_{4}$ and the metallic ferromagnets CuCr$_{2}$S$_{4}$ and CuCr$_{2}$Se$_{4}$ to clarify the electronic states responsible for the ferromagnetism on each site of the Cr spinel chalcogenides.

The experiment was done at beamline NE1B of the Accumulation Ring at High Energy Accelerator Research Organization (KEK). The Cr 2p X-ray absorption and MCD spectra show that the d-electron occupancies of the Cr atom in the Cu based Cr sulfide and selenide are not much different from that in the CdCr$_{2}$Se$_{4}$ in spite of the different formal valencies, Cr$^{3.5+}$ and Cr^{3+}, respectively. The observed Cu 2p MCD spectra show the existence of small magnetic moments on the Cu sites which are alingned antiparallel to the Cr 3d moment in CuCr$_{2}$S$_{4}$ and CuCr$_{2}$Se$_{4}$, consistent with band-structure calculation.

Precise Interferometric Measurements of the Dispersion at the K- and L-absorption edges of Nickel*

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Novel interferometers have been developed at the Mainz Microtron MAMI with which the complex index of refraction of thin self supporting foils can be measured. They are based on the coherence of two wave trains which are emitted if the low emittance 855 MeV electron beam of MAMI passes either through two foils or two undulators the relative distance of which is variable.

The interferometer in the x-ray region above a few keV consists of two foils from which transition radiation is emitted, a flat single crystal in Bragg geometry as energy selective element, and a pn-CCD photon detector [1]. Interference oscillations have been observed as a function of the distance between a 10 microns thick beryllium foil .and the 2 microns thick sample foil at the K-absorption edge of nickel at 8.34 keV. The extracted dispersion of Ni agrees well with the Kramers-Kronig transform of absorption measurements in the K-edge region and tabulated calculations elsewhere [2]. Our results will be compared with measurements of Bonse et al. [3].

The interferometer in the VUV and soft x-ray region consists of two collinear undulators between, for the current investigation, a 83.2 microgram/cm^2 nickel foil was placed, and a grating spectrometer [4]. High resolution measurements at the L_III-absorption edge around 855 eV reveal a very large negative atomic scattering factor f_1=-39.9+/-2.0, and a large positive f_2=65.4+/-2.8, to be compared with the 28 electrons of nickel. The Kramers-Kronig transform of the simultaneously measured f_2(omega) is in good agreement with the measured f_1(omega).

Work supported by the Deutsche Forschungsgemeinschaft DFG under contract No. Ba1336/1-1, and the Bundesministerium fuer Bildung und Forschung under contract No. 06 MZ 863 I TP2.

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HREELS investigation of Rotaxane thin films : structural, vibrational and electronic properties of mechanically threaded rings adsorbed on Au(111).

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The Nitrone Rotaxane (NOROT) is a molecular system consisting of a ring -the benzylic amide macrocycle- threaded on a twofold functionalised axis terminated by bulky stopper groups at both ends. As the benzylic amide [2]catenane -in which two macrocycles are threaded like the rings of a chain- these systems are seen more and more as key elements in the development of nanoscale devices such as molecular shuttles, switches and information storage systems. Their unique architecture, due to intra- and intermolecular hydrogen bonds, confers upon them unusual dynamic properties : the ring can rotate and shuttle back and forth along the thread through external stimuli. Thus, the behaviour of such complex molecules on a solid support and their two dimensional ordered arrangement are of considerable interest.

NOROT and NOROT thread thin films adsorbed on Au(111) were characterized using high resolution electron energy loss spectroscopy. The films order and their vibrational properties were explored as a function of coverage and preparation mode. Gas phase adsorption leads to the formation of overlayers with domain size larger than 100Å. In the case of ordered films, the intensity of out-of-plane C-H deformation mode relative to the in-plane C-H stretch indicates an adsorption geometry with the plane of the phenyl rings largely parallel to the Au(111) surface. Nevertheless, no chemisorption by the way of a Au-O bond appears for the NOROT as it was observed in the case of the macrocycle and the Fumaramide Rotaxane in which the two nitroxide functions are replaced by two amide groups on the thread.[1] The adsorption geometry of the rotaxane, the competitive adsorbate/adsorbate and adsorbate/substrate interactions, and the growth mode of the films will be discussed and compared with those of each component part -thread and macrocycle- and of the Fumaramide Rotaxane[1].

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THE ROLE OF BENZYLIC AMIDE MACROCYCLE IN THE ADSORPTION OF THE FUMARAMIDE ROTAXANE ON Au(111).

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Rotaxanes are a class of molecules composed of a ring (the macrocycle) which is threaded onto a bar (the thread) with stoppers at both end. These macromolecular structures are seen more and more as key elements in the development of nanoscale devices as molecular shuttles, switches and information storage system. The "mechanical bond" which holds the components of the molecules together is dynamic and can be used to modify a molecule's properties through external stimuli. Then, of interest is the development of techniques to grow two dimensional ordered arrays of these molecules such that they are still able to move.

A study on the adsorption of Fumaramide Rotaxane and its component parts (thread and macrocycle) on solid subtrate has demonstrated a key role of the macrocycle in the adsorbtion of the molecule together. Adsorption of the macrocycle from the gas phase on Au(111) has been investigated using high resolution electron energy loss spectroscopy (HREELS) and monochromated X-ray photoelectron spectroscopy (XPS). Quantification in terms of the relative amounts of carbon, nitrogen and oxygen, as determinated by XPS, are consistent with the formation of intact molecular species. The properties of the adsorbed species were explored as a function of increasing coverage and method of adlayer preparation. Changes in vibrational spectra and variations in core level binding energies and intensities provide insight into the thin film growth mechanism, in particular establishing that the nature of the bonding between the substrate and the adlayer at sub-monolayer and monolayer coverage involves chemisorption while at higer coverages (>monolayer) adsorbate-adsorbate interactions dominate. Based upon the vibrational results, an adsorption geometry with the plane of the phenyl rings parallel to the surface is favoured for a monolayer coverage, and the comparison with the vibrational results for the rotaxane and the thread indicates an important contribute of the macrocycle in the adsorption of the Fumaramide Rotaxane.

Coherence and correlation effects in the photoionization of Ne^+ $2s2p^5$ nl satellite states

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The study of photoelectron satellite lines has attracted a lot of attention because they provide detailed information on the dynamics of many-electron interactions. The case of the Ne^+ $2s2p^5$ nl satellite states is challenging because these states are embedded in the $Ne2^+$ continuum and several low energy Auger lines, providing evidence of their decay, have been detected[1]. The near-threshold study of these states allows to tackle two amongst the more debated topics in atomic physics: electron correlation and coherence. The latter manifests itself in strong interference effects whenever different paths lead to the same final state.

We have studied the Ne^+ $2s2p^5$nl satellite states via a series of photoelectron spectroscopy experiments from threshold up to a few eV above it. In the experiments the photoelectron energy was fixed and the photon energy was varied over the region of interest. When the photoelectron energy is made equal to "zero" then a threshold photoelectron spectrum (TPES) is collected. The experiments have been performed at the SRS Daresbury, but the high resolution TPES that has been measured, with the same spectrometer, at the Gas-Phase beam-line of the Elettra storage ring.

Due to the high resolution in both the exciting radiation and the threshold spectrometer a wealth of new features have been observed in the TPES spectrum. For example $2s2p^5$np states with a symmetry different from the ^2S one, observed in previous experiments [2,3], are clearly visible in the spectra near threshold. Moreover several peaks in the spectrum display interesting broadenings that result from their intrinsic linewidths and the effects of the final state interaction (Post Collision Interaction, PCI).

In the selected case of the $2s2p^5(^1P)3p$ state a clear change in the shape as well as in the intensity of the peak has been observed at a photoelectron energy of 2 eV. This has been interpreted as the manifestation of an interference effect between two channels leading to the same final state of the doubly charged ion. These effects have been predicted [4] and observed [5,6] in photoelectron-Auger electron coincidence measurements. To our knowledge this is the first time that evidence of this effect is provided by a non-coincidence experiment.

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Core level broadening in alloys: a controversial new link between electron spectroscopy and first principles theory

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The electrostatic energy of arrays of charges has attracted attention since the work of Madelung. However "charge transfer" is not a quantum mechanical observable and the fact that electrons are indistinguishable means that even if the electron density in a material is completely specified it is still not possible to associate a particular charge with a particular atom. This lack of an agreed definition has limited the usefulness of the concept of charge transfer.

In this work a new method of defining and measuring charge transfer based on the results of electron spectroscopy measurements is described. The method is applied to recent results obtained for the CuPd, CuPt and CuZn alloy systems including the first observation of "disorder broadening" of core level photoelectron lines in alloys by the effects of charge transfer [1]. The interpretation of the results is controversial [2,3].

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RAS: A new probe of surface states in ambient conditions.

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The combination of theoretical work, photoelectron spectroscopy and inverse photoemission has lead to a good understanding of surface states on metal surfaces. A number of occupied and unoccupied surfaces states on low index faces of metal single crystal have now been well characterized and they have been shown to have an important influence on the behaviour of such surfaces.

Recently a new optical technique, reflection anisotropy spectroscopy (RAS), has been shown to be very sensitive to surface states. RAS achieves surface sensitivity by measuring the change in polariastion on reflection of normal incidence light from a single crystal surface and transitions between surface states are prominent in the RAS spectra of Cu, Ag and Au. In this work the link between RAS and surface states will be explored and examples will be given of how RAS can be used to extend the study of surface states into the high pressure and electrochemical environments.

XPS and XAES study of carbon and fluorinated grafite materials

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X-ray -induced Auger spectra have been used for an investigation of the distribution of electronic density in the valence band. The Auger spectra have been represented as self-convolution of DOS modulated by Auger matrix element over the valence band. The DOS has been restored with an iteration regularization technique. The obtained results were compared with the experimental X-ray emission C K spectra, XPS of the valence band and quantum chemical calculations of the electronic structure. It has been obtained the C 2p LDOS for graphite, graphite monofluoride and the multilayer carbon nanotube samples synthesized at various conditions. For graphite monofluoride it has been calculated the interaction energy of holes in the final state.

In the next part it has been presented the results of studies of FGIC based on C2F with various guest molecules by XPS. These interstitial layered compounds were obtained in the conditions of low-temperature synthesis at temperatures less than 273 K by fluorination of graphite with liquid halogen fluorides using sequential exchange reactions. Most of the studied guest molecules interacted with matrix through Van der Waals forces, but there are experimental evidences of chemical interaction. For example, at implantation of pyridine a chemical interaction with matrix and formation of fluorination products take place within the interlayer spaces. It results to "defluorination" of the matrix and the increase of the ratio C/F. It has been proposed the formation of N-fluoropyridine cations which is promising fluorination agent. Other example is FGIC with Pd(II) acetylacetonate. It was demonstrared that in heating at H2 atmosphere the reduction of Pd(II) ions to Pd(0) state occurs between matrix layers.

PbS self-assembled dots on InP(110)

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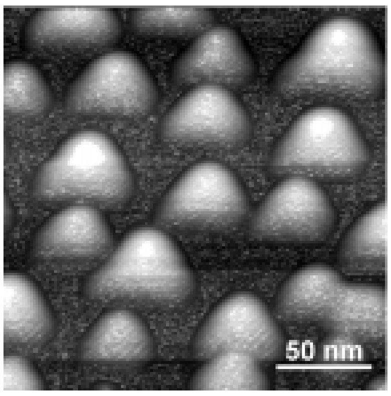
For the first time the MBE-growth of self-assembled PbS islands at the PbS/InP(110) interface is observed. By this example we introduce a new method of formation of nanostructures at semiconductor interfaces. The key point is to take advantage of different lattice structure of the constituents with the same lattice constants. PbS and InP have almost the same lattice constants but very different lattice structures (rocksalt and zincblende structure, respectively) providing a proper example of such situation.

XPS analysis shows that i) the growth probably occurs in the island mode and ii) the growth process is facilitated by sulfur - phosphorus exchange at the InP surface. From XPD and LEED it can be concluded that PbS islands are tilted with a characteristic angle of 20° between the InP(110) surface and the PbS(001) face. This tilt occurs along the [001] direction of the substrate as a result of transformation of the interface from partially incommensurable to lattice-matched one in this direction. This fact implies that the PbS(1-14) face matches the InP(110) substrate. AFM study of the PbS islands provides a good evidence for their self-ordering and shows that they typically have triangular lateral shape (figure). PbS islands with the size from 10 to 40 nm can be formed depending on substrate temperature and amount of deposited material. The mechanism of the growth and self-assembly is very different from the widely known mechanism of the formation of coherent quantum dots at the III-V/III-V and II-VI/II-VI semiconductor interfaces.

Apart from the formation of PbS dots, PbS single-crystal epitaxial layers can be grown on InP(110). Angle-resolved UPS provides information on structural quality and orientation of these films, as well as on the development of their electronic structure with increasing thickness. XPD and LEED data confirm the results on the PbS film structure.



ELECTRON SPECTROSCOPIC STUIDES OF STRIPE CORRELATIONS IN OXIDE SUPERCONDUCTORS

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In this paper, X-ray Absorption Near Edge Structure (XANES) and X-ray Photolelctron Spectroscopies (XPS) studies in Y-Ba-Cu-O and Nd-Cu-O systems with oxygen and 3d element doping backed by model calculations will be presented. These studies serves to provide the answers to the conjectures thrown and origin of spatial modulations related to superconductivity in the oxide superconductors. These aspects will be discussed in detail in this presentation.

Crystal-field splitting in CeB$_6$ observed by ultrahigh-resolution photoemission spectroscopy

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We have performed ultrahigh-resolution (DeltaE ~ 7 meV) photoemission spectroscopy (UHR-PES) on CeB$_6$ to study the electronic structure near the Fermi level (EF). Cerium atoms CeB$_6$ take a trivalent ionic state (Ce$^3+$) with one localized 4f electron. In the cubic crystal structure of CeB$_6$, the sixfold degenerate ground state 4f^1 (J=5/2) of Ce$^3+$ is expected to split into a Ganma7 doublet and a Ganma8 quartet, with the Ganma8 state being located at a higher binding energy. The UHR-PES spectrum shows a characteristic satellite structure at 270 meV binding energy due to the spin-orbit splitting of a Ce 4f electron (4f7/2), while the Kondo resonance peak (4f5/2), as usually seen in other Ce-compounds, is not clearly observed because of the relatively small Kondo temperature of CeB$_6$ (T$_K$<1K). Besides the spin-orbit satellite at 270 meV, we clearly observed an additional small structure around 70 meV from EF. Numerical simulations based on the single-impurity Anderson model with the noncrossing approximation show that this satellite is due to the crystal-field splitting (Ganma8 and Ganma7) of Ce 4f5/2 states in CeB$_6$. We discuss the obtained microscopic physical parameters for Kondo temperature and crystal-field excitation energy in comparison with the inelastic-neutron measurement as well as with the thermodynamic properties.

Ultrahigh-resolution photoemission study of CePd$_3$: absence of Kondo-insulator gap

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CePd$_3$ has been long believed as a typical Kondo metal, as evident from the T^2-dependence of electrical resistivity at low temperature. However, a recent optical conductivity measurement of CePd$_3$[1] has raised a question on this picture and proposed CePd$_3$ being a Kondo insulator which has a small energy gap (or pseudogap) at the Fermi level (EF) at low temperature. Indeed, the reported optical conductivity spectrum exhibits a remarkable temperature-dependent depletion from 0 to 1000 cm-1 (~100 meV) at low temperature. In order to examine this possibility more directly, we have performed ultrahigh-resolution (DeltaE~7 meV) photoemission spectroscopy (PES) on CePd$_3$. The valence band spectrum shows three main structures at about 1.5, 3 and 4 eV binding energy, which are ascribed to the 4f^1 final states, Pd 4d states, and 4f^0 final states, respectively. In the vicinity of EF, on the other hand, we found a small but very sharp peak just at EF and a hump at about 300 meV, which are assigned to the tail of Kondo resonance states and its spin-orbit satellite. Precise temperature-dependent PES measurements near EF have revealed that (1) there is no depletion in the PES spectral weight near EF in contrast to the case of "Kondo insulators" CeRhSb[2] and Ce$_3$Bi$_4$Pt$_3$[3] and (2) there exists a large peak (namely Kondo peak) across EF indicative of the metallic nature. All these PES results strongly indicate that CPd$_3$ is a conventional Kondo metal as suggested by many thermodynamic properties.

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Angle-resolved photoemission study of quasi one-dimensional conductor Nb_3Te_4

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We have performed ultrahigh-resolution (ΔE~15 meV, Δθ~0.3Åã) angle-resolved photoemission spectroscopy (ARPES) on a quasi one-dimensional (1D) conductor Nb3Te4, which has three zig-zag Nb chains along c-axis in the hexagonal units cell and exhibits a charge-density-wave (CDW) transition at 110K. We have succeeded in mapping out the band dispersions parallel (ΓA direction in the Brillouin zone) and perpendicular (ΓM direction) to the chain. We found several highly dispersive bands in the whole valence-band region along the chain, while the bands perpendicular to the chain are in general less dispersive, reflecting the 1D nature of the compound. In the vicinity of the Fermi level (EF), we found a dispersive band along the chain direction which clearly crosses E_F midway between Γ and A point in the Brillouin zone. According to the band calculation, this band is assigned to the Nb 4d band which forms a cylindrical Fermi surface along the chain direction. We found that the ARPES intensity of this Nb 4d band is substantially suppressed compared with the other bands far away from EF. This clearly shows the Tomonaga-Luttinger liquid behavior of 1D metallic Nb_3Te_4, where a quasiparticle states near E_F (or k_F; Fermi vector) is expected to be strongly suppressed. However, we have also observed a small Fermi-edge cutoff for this Nb 4d band, indicative of admixture of 2D or 3D nature in the Nb 4d band due to a finite interchain interaction in the crystal. We did not observed a clear spectral change across the CDW transition temperature. This may indicate that the present energy resolution (ΔE~15 meV) is not enough to see it and/or that the nesting area on the Fermi surface is too small to find with the present angular resolution (Δθ~0.3Åã).

Unified View of Chemical Interaction and Surface Magnetism in Co Films on Different Passivated GaAs Surfaces Studied by Photoemission Spectroscopy

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The hybrid system consisting of a ferromagnetic thin film on semiconducting surface is considered to be unique to innovate the non-volatile magnetotransport-based electronic devices [1]. There is a lot of interest to study the surfactant effect of VI-elements, such as Se, S and O for transition metal epitaxy on semiconducting surfaces, such as GaAs.

Recently we have performed a series of photoemission measurements for Co films on different passivated GaAs, such as Se/GaAs(001), S/GaAs(001) and GaO/GaAs(001), as well as on bare GaAs(001). For all the passivated surfaces, the As-free Co film surface has been obtained. This finding is very different from the system like Co on bare GaAs, in which As-rich film surface is formed. During Co deposition, it was found that S and Se were segregated at top of Co films on S/GaAs and Se/GaAs. But, O was remained at interface for Co on GaO/GaAs. At the same time, nature of chemical interaction at initial stage of deposition was found to be different depending passivated substrate.

In order to study the magnetic phase of Co films on GaAs, magnetic linear dichroism in angular distribution (MLDAD) measurement in surface sensitive photoemission was performed. Under the same experimental condition, the peak-to-peak intensity in MLDAD spectra was found to be 0.7% for Co(~27 ML, monolayer)/Se/GaAs, 2.5% for Co(~27 ML)/GaO/GaAs and 7.4% for Co(~20 ML)/S/GaAs. The MLDAD results manifest that the magnetic ordering in Co film is dependent on properties of substrate. For example, in spite of formation of amorphous Co film on GaO/GaAs, the surface was found to be ferromagnetic. But degree of magnetic ordering is relatively lower than that of Co on S/GaAs.

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Study of Correlation-Induced Satellite Structure in Co2p Photoemission Spectra for Co Films as a Function of Thickness

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Satellite structures in the photoemission spectra for 3*d*-transition metals have been frequently reported [1]. The well-known examples are 6 eV-satellite in Ni valence band and core level photoemission [2]. In the case of a thin film system, it is now established that both *d*-*d* interaction and adatom-substrate hybridization play important role for originating satellite. The reduction of dimension sometimes enhances *d*-*d* interaction along the surface normal. By taking the consideration of *d*-*d* interaction and hybridization, we examined Co2*p* satellite structure, which is usually non-visible for bulk system, in Co film for different thickness.

For our experiment, we deposited Co films on Cu(001) and O-rich Cu(001). In the case of Co films on Cu, we observed a distinct difference in intensity around the satellite region in Co2*p* photoemission spectra as thickness is varied. For example, in a 1 ML (monolayer) film, satellite is more intense than that in other films such as 3 ML or 5 ML. The reasons for intense satellite are the strong *d*-*d* interaction and less hybridization in 1 ML film. On the other hand, in a 1 ML Co film on O-rich Cu, we observed even more intense satellite structure than that in same one on Cu. This difference in two systems may have been arisen from the geometrical shape of films. In the case of 1 ML film on Cu, film consists of scattered 1 ML- and 2 ML-high islands. On the other hand, we predict that, due to oxygen surfactant effect, a 1 ML Co film on O-rich Cu consists of well-shaped 1 ML-high islands with higher density. This situation in film on O-rich Cu may reduce the hybridization strength and increase the *d*-*d* interaction, as well.

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Observation of Ga 3d Two-Hole States from GaAs Surfaces

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Satellite structures and their resonant enhancement observed in photoemission spectroscopy of strongly correlated systems have attracted much interest. However, these phenomena have not been applied to studies of semiconductor surfaces. In this study, the Ga 3d two-hole states were observed from GaAs(001)-c(4x4), -2x4, (110)-1x1, and (111)A-2x2 surfaces using resonant photoemission spectroscopy. The intensities and the energy positions of the surface components of the two-hole states were analyzed.

Experiments were performed using a combined system of photoemission analysis chamber and a molecular beam epitaxy (MBE) growth chamber, connected to the beamline BL-1C in the Photon Factory of the High Energy Accelerator Research Institute.

The Ga 3d two-hole final states appeared when the photon energy was tuned to near the 3p absorption threshold (about 106 eV) [1]. Multiplet terms ^1G, ^1D, and ^3F were clearly distinguished. The effective Coulomb repulsion between the two 3d holes was estimated to be 11.6 eV for the ^1G term. The Slater integrals F^2 and F^4 were determined to be 14.4 and 6.0 from the relative energy positions of the multiplet terms. In addition, the surface components of the two-hole states were observed in the spectra of the (001)-2x4, (110)-1x1, and (111)A-2x2 surfaces having Ga atoms at the surfaces. The curve-fitting analysis revealed that the intensities of the surface component of the two-hole states were considerably smaller than those of the d^9 states. This is ascribed to the reduced absorption probabilities of the 3p electrons at the surfaces because the Ga dangling bonds at the surface have a predominantly p character due to the surface relaxation.

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Local Geometry and Electronic Structure of $\mathrm{Al}_{90}\mathrm{Fe}_{x}\mathrm{Ce\$}_{10\text{-}x}$ and

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The x-ray absorption near edge structure (XANES) above the Al K-edge in Al$_90$Fe$_3$Ce$_7$, Al$_90$Fe$_5$Ce$_5$, Al$_90$Fe$_7$Ce$_3$ and Al$_90$Co$_10$ has been measured at the Stanford Synchrotron Radiation Laboratory (SSRL), using the JUMBO monochromator equipped with YB$_66$ crystals. The resolution of the YB$_66$ crystals at 1550 eV is 0.46 eV. Theoretical "ab initio" full multiple-scattering analysis of the XANES data on the basis of original G4XANES package has been done. Comparison of experimental data with theoretical results allowed us to choose the best structural models for the Al site in the alloys under study. For example the structure of Al90Co10 alloy is well reproduced by the Al$_5$Co$_2$ alloy. We also investigated the electronic structure of these alloys and peculiarities of localized correlated Ce 3d states and band-like Al p-states and Co(Fe) p-states hybridization. We found that this interaction of unoccupied electronic states has specific character, namely, Al as well as Co (Fe) p-states are pushed by Ce d states from the energy interval of their localization. Since the dipole transition matrix element for the Al K-edgs does not vary sharply with energy, the experimental XANES for the Al K-edges can be used for probing the partial Al p p unoccupied states in the conduction bands of these alloys

Observations of Surface Core-Exciton and its Decay on Solid Xe.

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The Excitation and the decay of Xe5d level of solid Xe have been investigated using partial electron yield spectroscopy and photoelectron spectroscopy with synchrotron radiation. Surface-sensitivity of the absorption spectrum was achieved by monitoring the partial electron yield. We found that the photon energy corresponding to the excitation of the Xe5d->6p (core exciton) at the surface to differ by -0.2 eV from the one in the bulk. This surface-to-bulk shift can be attributed to a difference in the screening efficiency of the Coulomb interactions between the hole at Xe5d and the electron at the Xe6p level at the surface compared to that in the bulk. The decay of the exciton is investigated in detail. The result contrasts to the decay spectrum of the Ar2p core exciton as observed on solid Ar[1]. The difference between Xe (5d->6p) and Ar (2p->4s) is discussed and we suggest that it may be related to the fact that Ar4s is the lowest unoccupied level while Xe6p does not meet this condition.

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Electronic properties of (C60, K)/Si(111) systems studied by electron energy loss spectroscopy

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Since the discovery of superconductivity in K_3C_{60}, alkali or alkali-earth metal doped fullerenes have been studied extensively. In K_3C_{60}, three electrons transfer from K atoms to one C_{60} molecule. On the other hand, we researched C_{60} molecules adsorbed on various metal and semiconductor surfaces using electron energy loss spectroscopy (EELS). We have reported charge transfer from the surface to C_{60} molecules in a C_{60} monolayer on a Si(111)7×7 substrate or on a Si(111)√3×√3-Ag substrate. [1] In this manner, K-doping and the existence of the surface have a same role in the view point that they affect the electronic structure of C_{60} molecules. It is significant to investigate what happens to C_{60} molecules when K-doping and a Si(111)7×7 surface coexist.Å@Å@ We studied electronic structures of C_{60} monolayer films on a Si(111)δ7×7-K, and on Si(111)3×1-K surface using EELS. A K-doped C_{60} monolayer film on a Si(111)7×7 was also investigated for comparison. A Change in the EEL spectrum of a C_{60} monolayer film on the Si(111)7×7 substrate along with increase of entered K atoms is quite different from that of KxC_{60}. This indicates that interactions between C_{60} molecules and the Si(111)7×7 surface is strong, and that the existence of the surface makes the difference of the change in the EEL spectrum. It was also revealed that interactions between C_{60} molecules and the Si(111)δ7×7-K surface as well as Si(111)3×1-K have ionic character. Amount of charge transfer from the Si(111)δ7×7 substrate to C_{60} molecules is larger than that from Si(111)3×1-K to C_{60} molecules. Comparing EEL spectra of K-doped C_{60}/Si(111)7×7 and that of C_{60}/Si(111)δ7×7-K, it was revealed that K atoms adsorb on dangling bonds of the Si(111)7×7 surface in the initial process of K-doping into the C_{60} monolayer film on the Si(111)7×7 substrate.

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Novel type of X-Ray monochromator for XPS laboratory systems: Pseudo-Spherical Multi-Stepped

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Modern XPS techniques need both good spectral resolution and the largest possible value of the x-ray monochromator throughput. Conventional focusing technique made by plain, cylindrically or doubly curved (on spherical or toroidal surface) crystal monochromators does not allow to reach high resolution without significant losses in the transmission function. Here a novel type of the x-ray monochromator based on the special shape of reflecting surface - pseudo-spherical stepped [1] is proposed. As a prototype for theoretical simulation x-ray monochromator with 0.5 m focusing circle of VG Multilab ESCA 2000 (3000) system has been used. X-ray tracing has been performed for Al K alpha (E=1.487 eV) radiation reflected by quartz (10-10) crystal surface at 0.65 eV spectral resolution. It has been demonstrated that using proposed multi-stepped device one can expect the gain of 3-5 times in the throughput of the monochromatized radiation without the losses of spectral resolution, if increase the length of diffracting element up to 200 mm.

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Self-organized quantum wires on semiconductor surfaces: the new frontier provided by reduced dimensionality

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Recently we have searched for the possible exotic physical properties of the nanostructures formed on semiconductor surfaces by STM and high-resolution photoelectron spectroscopy/diffraction. The major objects have been the 1D quantum wires (QWs), 2D overlayers, and ultrathin films on Si and SiC surfaces. In the present talk, one of these projects, the study of the well-ordered surface phases composed of self-organized QWs on Si and SiC surfaces is reviewed. The electronic band structures of these surfaces are emphasized in understanding the formation of QWs and low-dimensional physical properties.

Three different types of QWs are studied. The metastable QWs of group-III (Al and In) and group-IV (Pb) adsorbates on the Si(001)2x1 surface were known to form the so-called parallel-dimer structure and the 2xn (n = 2, 3 and 5) phases. The surface band structures observed, however, suggest that there is no obvious 1D electronic coupling [1]. The QW formation, then, can be understood in terms of a very local mechanism such as the 'surface polymerization'. The highly-stable Si QWs were observed on the Si-rich SiC(001) surface to form the nx2 (n = 3, 5, 7, 8, and 9) phases. The surface-state bands exhibit very little dispersions indicating strong localization of the surface electrons [2] without any 1D electronic coupling. An interesting and intriguing 0D fluctuation of unit cells are revealed by STM, which is thought be due to the '0D electronic decoupling'. I finally discuss the metallic In QWs formed on the Si(111) surface. The 4x1-In surface was known to have 1D metallic surface states and we have predicted and found a reversible transition, of Peierls type, into a semiconducting phase [3]. The 1D CDW and periodic-lattice-distortion (with a doubled periodicity) along the QWs is observed directly by STM at low temperature. The Fermi contours of the metallic phase exhibit a perfect nesting predicting precisely the CDW periodicity.

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Local and Electronic Structure of small free NaCl clusters *

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X-ray absorption fine structure of small free NaCl clusters above Cl L $_{2,3}$ and Na K-edges has been measured at BW# beamline of DESY (Hamburg). Theoretical "ab initio" analysis of x-ray absorption at Cl $L_{2,3}$ edge and Na K-edge have been done using original G4XANES software package [1] based on a full multiple-scattering theory. All main factors that cause the broadening of the spectra (i.e. final lifetime of core hole, limitations of mean free path of photoelectron and, also, experimental resolution) have been taken into account and all of these factors were contributing to imaginary part of complex potential used.

To study small free cluster geometry XANES spectra have been simulated for the following models: 1) as a fragments of cubic (NaCl -like) crystal lattice with Na-Cl interatomic distances (2.82 Å) equal to the distances from infinite crystal, 2) as a fragments of cubic (NaCl -like) crystal lattice, but with smaller (2.5 Å) Na-Cl interatomic distances, equal to these ones obtained from pure theoretical approach based on the minimisation of free cluster full energy [2], and 3) and 4) distorted non-cubic clusters, with geometry obtained from theoretical approach in Ref. 2. and Ref. 3. The comparison of theoretically simulated spectra with experimental one shows that interatomic Na-Cl distance varies significantly, starting from biatomic cluster (NaCl molecule) to eight-atomic cluster (Na_4Cl_4 "cube") and finally to large clusters, converging to infinite solid. The results obtained also strongly support the evidence for a distortion of free cluster geometry from pure cubic.

The present approach let us also to investigate the peculiarities of Na_4Cl_4 small cluster electronic structure. The distribution of unoccupied partial *s*-, *p*- and *d*- electronic states has been obtained. Density of states analysis allows one to study the details of chemical bonding in small NaCl clusters.

* Work is supported by joint grant of RFBR (Russia) and DFG (Germany).

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Bulk 4f Electronic States of CeNiSn and CePdSn Probed by HIGH-RESOLUTION Ce 3d-4f RESONANCE PHOTOEMISSION

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In order to clarify bulk 4f electronic states of a Kondo semiconductor CeNiSn, we have measured Ce 3d-4f resonance photoemission (RPES) spectra of CeNiSn and its reference material CePdSn with unprecedented high resolution (100 meV at the photon energies of about 880 eV) at a twin-helical undulator beamline BL25SU in SPring-8[1]. The Ce 3d-4f RPES mainly reflects bulk 4f states[2] due to a longer photoelectron mean free path compared with the 4d-4f RPES. The obtained 3d-4f on-resonance spectra show a clear doublet structure consisting of a tail of the Kondo peak ($f_{5/2}^1$ final state) and its spin-orbit partner ($f_{7/2}^1$ final state) for both materials. The intensity of the $f_{5/2}^1$ final state is stronger than that of the $f_{7/2}^1$ final state in the 3d-4f RPES spectra of CeNiSn while the $f_{5/2}^1$ final state is weak for CePdSn. Both 3d-4f and "surface-sensitive" 4d-4f RPES experimental spectra are well fitted by the spectral calculations based on a single impurity Anderson model with considering the bulk and less hybridized surface components. The calculation also gives a reasonable value of the Kondo temperature for CeNiSn. The 3d-4f off-resonance spectra ("non-4f" spectra) are properly reproduced by band-structure calculations for both compounds.

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Abstract # 747
Program#

Electron scattering resonance and the free electron density of states in solids*

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In gas-phase electron-energy loss spectroscopy, electron resonances in molecules are indicated by selective excitation of fundamental, overtone, and combination vibrations, as well as strong variation in the incident energy dependence of the corresponding scattered electron intensities. In the condensed phase several new effects due to multiple elastic and inelastic electron scatterings can give structures within an existing vibrational excitation function. In an ordered solid, the conduction band density of states (CB DOS), which stems from the band structure, is defined whenever a quantity that depends on the electron wave vector through E(k) is averaged over all directions of 'k'. The role of the CB DOS for electron scattering in the condensed phase is investigated with electron-energy-loss spectroscopy of molecular oxygen embedded in an Ar matrix. Actually, oxygen in the gas phase offers smooth resonant vibrational cross sections[1] spanning most of the energy range where the CB DOS of solid Ar is known[2]. In contrast to its gas-phase counterpart, the resulting vibrational energy loss intensities of matrix isolated oxygen exhibit strong variations as a function of the incident energy[3]. Except for a relative change in intensity, these variations remain essentially at the same energy for different scattering angles and follow the inverse of the CB DOS. It is shown that under resonant scattering conditions this behavior arises more specifically from changes in the resonance lifetime due to variations in the CB DOS of the host medium.

*This research was sponsored by the Medical Research Council of Canada.

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ELECTRONIC STRUCTURES OF ELECTRON-DOPED MANGANITE: $La_{0.7}Ce_{0.3}MnO_3$

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The electron-doped $La_{0.7}Ce_{0.3}MnO_3$ (LCeMO) manganese perovskite exhibits the metal-insulator (M-I) and ferromagnetic transitions, with the concomitant colossal magneto resistive (CMR) phenomenon. The electronic structure of LceMO has been investigated by performing the band calculations under the local spin density functional approximation (LSDA), which are then compared to the photoemission spectroscopy (PES) data. The partial density of states (PDOS) of LCeMO, obtained from the LSDA calculations, does not agree with the measured Mn 3d photoemission spectrum. This is in contrast to the hole-doped CMR perovskites that reveal rather good agreement between experiment and theory. In order to investigate the effect of the Mn 3d on-site Coulomb correlation in the electronic structure of LCeMO, we have calculated the Mn 3d quasi-particle spectral density by performing the LSDA+U calculations. Our calculations show that the Mn 3d on-site Coulomb correlation accounts for the major features in the experimental PES spectra, such as the peak positions and the reduced spectral weight near the Fermi level.