Microlocalization of Gd in Cell Nuclei: Key for the Success of Brain Cancer Therapy

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^{157}Gd is a potential agent for neutron capture therapy (GdNCT), a brain cancer therapy never clinically tested. We directly observed the microdistribution of gadolinium in cultured human glioblastoma cells (in vitro) exposed to gadolinium-diethylene triamine pentaacetic acid (Gd-DTPA). We demonstrated, with three independent techniques (X-PEEM, ICP-MS and ToF-SIMS), that Gd-DTPA penetrates the plasma membrane, and we observed no effect on cell survival. A systematic microchemical analysis with X-PEEM revealed a higher Gd accumulation in cell nuclei compared to cytoplasm. Furthermore, we studied the microlocalization of Gd in brain cancer tissue sections, extracted from patients intraveneously injected with Gd-DTPA before surgery for tissue extraction. We found that also in this (in vivo) case Gd is preferentially accumulated in cell nuclei. This is significant for prospective GdNCT because the proximity of Gd to DNA increases the cell-killing potential of the short-range electrons emitted during the neutron capture reaction.

Angle resolved two-dimensional mapping of electron emission from Cl2 2p (L2,3) excitations.

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Angle resolved Auger and valence photoelectron spectra of Cl_2 were measured over 14 eV-wide photo energy range across the Cl_2 2p ionization thresholds. It was measured using highly efficient time-of-flight (TOF) spectrometers coupled with the undulator of the Atomic and Molecular beamline of the Advanced Light Source and advanced data acquisition system [1].

Auger electron spectra of $2p_{3/2,1/2} \rightarrow \sigma_g^*$ and $2p_{3/2,1/2} \rightarrow nl$ resonances were analyzed and the evolution of the resonant Auger to the normal Auger decay distorted by postcollision interaction was examined. Valence photoionization channels were shown to note resonate strongly at the photon energies of the core-to Rydberg excitation. That is in contrast to the strongly resonating ones seen in HCl molecule [1]. In addition, angular distribution of the photo- and Auger electron lines were derived. Analysis of the Auger decay of 2p electrons excited to the antibonding σg* orbital showed slower dissociation than in HCl [2] and mostly molecular character of the Auger decay.

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New Developments in the Theory of X-ray Absorption and Core Photoemission*

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There has been dramatic progress over the past decade both in theory and in ab initio calculations of x-ray absorption spectra (XAS) and core level x-ray photoemission spectroscopy (XPS). The theory of x-ray absorption fine structure (XAFS) is now reasonably well understood, and rapid progress is now being made in understanding x-ray absorption near-edge structure (XANES). This talk reviews the developments in this field by many groups leading up to the current state [1]. These developments have led to several ab initio codes which permit a quantitative interpretation of the spectra in terms of geometrical and electronic properties of a material. High-order multiple scattering (MS) theory can give an approximate treatment of XANES, but this approach can fail close to an edge, where full MS calculations are often necessary. Nevertheless a fully quantitative treatment of XANES remains challenging, due to a number of many-body effects, e.g., the approximate treatment of the core-hole, multiplet effects, the photoelectron self energy, and inelastic losses. Essentially the same underlying theory has be applied to a number of other spectroscopies such as XPS, anomalous x-ray scattering (AXS), DAFS (diffraction anomalous fine structure) and XMCD (x-ray magnetic circular dichroism). These developments are illustrated with a number of applications.

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Non-dipolar and Dipolar Angular Distribution of S $2s$ and $2p$ of SF$_6$ Core-Level Photoionization in the Vicinity of F $1s$ Excitation*

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In this work, angular distributions of S $2s$ and $2p$ photoelectrons of SF$_6$ were measured in the vicinity of F $1s$ (t_{1u} to ${a*}_{1g}$) excitation with time-of flight spectrometers [1] at the undulator beamline 8.0 of the Advanced Light Source. Considerable variations were observed in the dipolar and non-dipolar anisotropic parameters when the excitation energy is tuned across the resonance. Those variations correspond to a relative-partial-cross-section change of 5% in $2p$ and, most unambiguously, of 15% or more in $2s$ non-dipolar geometry. Although the original intent of this work was inspired by the observation of MARPE effects [2] in solids, we consider the effects observed here in SF$_6$ relying more on the preferential excitation of F $1s$, which results in localised core hole only on the F-S-F axis parallel to the incident photon polarisation [3], than the mechanism of MARPE effects in the solids where at least the nearest as well as the next-nearest neighbours have to be summed over coherently in order to get more than 15% increase in the total photoionization cross section [4].

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The Effect of Deposition Pressure on Adsorbate Structure and Coverage: Oxygen on W(110)*

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In most prior surface science studies, it has been assumed that total exposure, rather than both pressure and time as independent variables, controls the types of adsorption structures formed. However, the potential importance of deposition pressure as a variable has recently been suggested in a study of the kinetics of the low pressure adsorption of oxygen on W(110) using time- and chemical-state-resolved photoelectron spectroscopy and diffraction.[1] As a more quantitative measure of such effects, we have used ultrahigh vacuum scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and X-ray photoelectron spectroscopy (XPS) to explore the adsorbate structures and the coverage dependence of oxygen on W(110) as a function of the deposition pressure and for room temperature exposures. For the same total adsorbate exposure in Langmuirs (L), our study shows that changes in deposition pressure of as little as a factor of 3 cause significant changes in the apparent structures, domain sizes (e.g., of (1x2)O), and the actual resulting coverages of the adsorbate layer in monolayers. Low pressure deposition (3 x 10^{-9} torr) for total exposures of 2-12L yields structures which do not show a distinct LEED pattern, but show small domains, ~2nm x 3nm, of local (1x2) ordering in the STM images and total coverage 0.13-0.17ML. Intermediate pressure deposition (10^{-8} torr) gives domain sizes of ~ 3-5nm with coverage of 0.15-0.3ML, while higher pressure (10^{-7} torr) gives structures with good LEED patterns and large well-ordered (1x2) and (2x2) domains in STM images. Total coverages derived from STM data using a software thresholding technique indicate that a critical dosing pressure exists for both the (1x2) and (2x2) structures, below which coverage does not increase with increasing exposure time. The coverage measurements were also confirmed by using XPS to compare the integrated areas of the O_{1s} and $W_{4p1/2}$ peaks. The inability to form complete monolayers of (1x2) and (2x2) structures at dosing pressures of 1 x 10^{-9} torr and 3 x 10^{-9} torr respectively indicates that an equilibrium condition has been reached, from which surface free energies for both of these structures can be derived.[2] Finally, in addition to the well-known ordered (1x2), (2x2), and (1x1) structures for O/W(110), we have characterized a new fourth ordered structure using LEED and STM. The structure formed for oxygen exposure of 3 to 6 L and coexisted with the (2x1) structure. The primitive unit cell is a perfect rectangle, 0.774nm x 1.368nm, with 15 W and 6 O atoms and has the matrix notation ((3,-1),(0,5)) relative to the W(110) substrate.

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A new application for Koopmans energies

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In the early developments of electron spectroscopy changes in the one electron Koopmans energies of core states of atoms in molecules and solids were related directly to environmental shifts observed in X-ray photoemission, but it was soon realised that final state relaxation effects were also important. Although the Koopmans energies are not diectly observable, this study shows how the variation of these one electron eigenvalues with lattice spacing provides a useful fingerprint of the bonding regime. Using the CRYSTAL self-consistent Hartree-Fock program Koopmans energy variations with lattice parameter are calculated for a range of alkali halides and oxides and compared with covalently bonded systems such as C(diamond),Si and Ge. In the ionic systems at large interionic spacings Madelung shifts relative to the free ion values (positive for the cations, negative for the anions) dominate, but around equilibrium separation a small additional homopolar contribution is identified.Under high compression both anion and cation eigenvalues experience positive repulsive shifts due to the enhanced electron density. In contrast when C,Si,and Ge atoms are brought together the eigenvalues initially increase relative to the free atom, but then reach a maximum before decreasing to values at equilibrium close to those of the free atoms : this variation is related to changes in hybrdisation pattern with atomic distance. The manner in which the core Koopmans energies respond to valence electron bonding gives general insights into trends in initial state contributions to photoemission and Auger shifts.

Electron Spectroscopy of Nanostructured Titanium Dioxide Materials for Solar Cell-, Battery-and Display Applications

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The properties of semiconductor surfaces in contact with liquid solutions and the processes occuring at such interfaces are of fundamental interest in a large number of areas in current applied surface chemical physics. The mechanisms of the processes involved are generally found to be highly dependent on the nature of the solid-liquid interface. The field of nanostructured transition metal oxide electrodes is quickly expanding since the demonstration of the usefulness of such electrodes in efficient photoelectrochemical solar cells [1]. A nanostructured electrode consists of interconnected nanocrystallites forming a porous structure (porosity around 50%). The significant property is the extremely large inner surface allowing for photoelectrochemical reactions to take place in the entire volume of the electrode. The solar cell is constructed via adsorption of dye molecules (in particular $RuL_2(SCN)_2$, where L=biisonicotinic acid) on the inner surface of nanostructured titanium dioxide, which act as "antennas" for solar light absorption leading to subsequent injection of electrons into the conduction band of titanium dioxide. The solar cell is only one of several potential applications of such electrodes. High charging capacities have also been reported of nanostructured anatase titanium dioxide electrodes when lithium is intercalated into the nanocrystals [2,3]. Lithium intercalation also exhibits electrochromic properties. Such a porous nanostructure can thus be employed both in battery and display applications. In addition, adsorption of electrochemically oxidizable or reducible molecular molecular species (e.g. triarylamine or viologens) can be used to construct a variety of display systems of different colors.

The present contribution reports recent results of electron spectroscopy on nanostructured films for the abovementioned applications. It is shown that information may be obtained both on structural and electronic properties which provides further understanding of the function of such films in actual devices.

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X-ray Absorption and Photoelectron Spectroscopy on Ice

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We have performed NEXAFS and XPS investigations of the surface and the near-surface region (0.5 micrometer) of ice and water at temperatures in the range from 173 K to 274 K. A newly developed high-pressure XPS and NEXAFS apparatus allows us to investigate the ice and water samples in equilibrium with their vapor (e.g. at pressures of up to several torr). Our NEXAFS measurements reveal that the ratio of ordered (ice-like) vs. disordered (water-like) regions in our polycrystalline ice samples is increased when approaching the melting point. The large escape depth of fluorescent photons in ice/water (about 0.5 micrometer) implies that the liquid-like layer is present throughout this depth range. This argument is supported by angle-of-incidence measurements. It is argued that, in addition to the liquid-like layer at the ice surface, there is also a liquid-like layer at the grain boundaries in polycrystalline ice.

Multi-Atom Resonances on the Re Valence Orbitals

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The np to nd resonance has been widely observed in the phtoemission study of atoms and solids. This resonance was viewed as an atomic or localized phenomenon, since the probability for such a resonance depends critically on the strength of configuration interaction, and therefore on the localization of the core-excited state [1,2].

However, Fadley and coworkers recently observed a very strong Mn2p to O1s resonance, in addition to the normal Mn2p to Mn3p resonance, for metal oxides, such as MnO [3]. This new observation was termed as the interatomic multi-atom resonant photoemission (MARPE) effect [3,4].

In this work, we report the variable energy valence level photoelectron spectra of $Re(CO)_5X$ (X=Cl and Br). We observe an intense Re 5p to 5d resonance not only on the Re 5d based orbitals, but also on the pure halogen based P_π orbitals. Our results present another example of the MARPE effect, but for organometallic complexes in the gas phase.

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Interference Effects between Auger- and Photoelectron in the Xenon N5O2,3O2,3Auger Decay *

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In 1994, Vegh and Macek [1] predicted strong interference effects between the emitted electrons from innershell photoionization and the subsequent Auger decay, when both electrons have the same kinetic energy, hence becoming indistinguishable. Since then several experiments have been performed to investigate these effects [2-5].

To observe these interference effects, the two equal energy electrons have to be detected in coincidence. The interference between the electrons appears in the enhancement or depression of the double photoionization Triple-Differential-Cross-Section (TDCS), depending on the final state, as seen by Selles et al. [4]. A more dramatic interference pattern has been predicted for the case where the photon energy resolution is less than the core hole lifetime width.

The experiment was performed at the high-resolution beamline 10 of the Advanced Light Source (ALS) in Berkeley using a set of electron time of flight detectors in coincidence. We concentrated on the case of Xe $N_5O_{2,3}O_{2,3}$ Auger decay leading to the $^1S_0$ doubly charged final state, where a strong destructive interference can be observed [2,3]. We will present some new data of the angular and kinetic energy dependence of the TDCS.

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Chemical Reactivity of Methylbenzenes from Core-Photoelectron Spectroscopy and Theory

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Electrophilic reactions are of fundamental interest in synthetic and mechanistic organic chemistry and of great importance in many industrial processes. The rate-determining step for electrophilic reactions involves the formation of a charged intermediate by addition of a positively charged species at a site in the molecule. Since core ionization involves the addition of a positive charge by removal of an electron, we expect that the chemical factors that influence these two properties will be the same, and that they are correlated. We have previously found that for ethene, propene and 2-methylpropene, there is a linear relationship between carbon 1s energies and activation energies as measured in the gas phase [1].

In order to investigate this relationship further, we have measured the C1s ionization energies for benzene and a series of methylated benzenes. The compounds comprise methylbenzene, 1,2-dimethylbenzene, 1,3-dimethylbenzene, 1,4-dimethylbenzene, and 1,3,5-trimethylbenzene. The spectra were measured in the gas phase using synchrotron radiation at beam line I411 at the MAX-II laboratory in Lund, Sweden. The excitation energy was 330 eV, about 40 eV above the threshold.

The ionization energies of the ring carbons were compared with experimental reactivity data for the mono- and dimethyl compounds. These are relative rates of replacements of tritium by hydrogen. The reactivity data show extreme position sensitivity of the ring carbons and provide a good test set for correlation with C1s energies. In addition, these replacement reactions are not considered to be influenced by sterical hindrance, which facilitate the comparison. The results show that the activation energies correlate well with the C1s energies and demonstrate that the relationship between reactivity and C1s energies found earlier in the gas phase also holds for reactions taking place in liquids.

The assignment of the spectra and subsequent analysis were based on ab initio calculations at the DFT level using Gaussian 94 and the equivalent-core approximation. The calculated chemical shifts are in good agreement with experimental values and were analyzed in terms of ground-state potential energies and final-state relaxation energies. The results confirm earlier findings [1] that the reactivity for the ring carbons is mainly due to the charge distribution in the ground state, and not to the different ability of the molecules to delocalize the added charge in the transition state.

XANES microspectroscopy of biominerals with photoconductive charge compensation

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Specimen charging under x-ray illumination is a well known phenomenon that can seriously obstruct the analysis of insulating samples [1]. Synchrotron X-PEEM spectromicroscopy can reach a lateral resolution of 20 nm, an order of magnitude less than electron microscopies, but has the added capacity to probe oxidation state through total yield x-ray absorption near edge structure (XANES) spectroscopy. This capability may be compromised, however, if specimen charging restricts electron emission, as was encountered in the study of silicified bacteria from an Icelandic hot spring microbial mat. Bacteria living in an environment containing a high concentration of dissolved silica provide nucleation sites for amorphous silicate precipitation, a process which may lead to the preservation of the cellular structure, i.e. fossilization. TEM studies of bacteria in progressive stages of mineralization showed mineral formation was initiated in the extracellular sheath, reaching the cell interior after death [2]. Spectromicroscopy at the Si L-edge of sectioned mineralized bacteria encountered major charging difficulties, which were relieved by simultaneously illminating the specimen with 325 nm HeCd laser light during the analysis. The low energy light excites mobile free electrons below the work function threshold, which can offset surface positive charge. This approach allowed spectroscopy to be performed from microscopic areas, and may be applicable to a wider range of insulating samples.

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Resonant Inelastic Soft-X-ray Scattering of La$_{1-x}$Sr$_x$CoO$_3$ at Co 2p edge

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Resonant soft-x-ray scattering measurements were performed on La$_{1-x}$Sr$_x$CoO$_3$ (x=0.0, 0.4, 0.9) at the Co 2p edge. Changes in inelastic scattering from valence band excitations on going from undoped to highly doped compounds were studied. Obtained spectral profiles reflect the high degree of covalency for Co-O chemical bonds in these compounds which increases with increasing x. For all the samples, the spectra reveal substantial contribution of normal Co 3d,4s-2p x-ray fluorescence. The reason for that is believed to be the band-like character of Co 3d states giving rise to efficient screening and significant charge-transfer between neighboring Co sites.

Particular attention was paid to the temperature dependence of LaCoO$_3$ spectra which were recorded at 90, 300, and 525 K. The largest changes in the spectra occur upon cooling rather than heating of the sample and are observed in the low-energy-loss range. The analysis of the results, based on both band-structure calculations and localized, many-body approach, suggest that the temperature-induced magnetic transition in LaCoO$_3$ around 100 K is a low-spin-to-intermediate-spin rather than low-spin-to-high-spin transition.

Imaging magnetic domains on a nanometerscale with Magnetic Transmission X-ray Microscopy

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The magnetism in systems of low dimensionality as e.g. ultrathin magnetic films or multilayered systems exhibits a scientific curiosity if the size of the objects approach characteristic lengths resembling the balance between exchange interaction and anisotropy energies. Furthermore there is also an increasing importance of such systems for future technological applications like magnetic sensors based on the giant magnetoresistance (GMR) effect, spin valve structures or tunneling junctions or magnetic nanostructures (MRAM technology) which can be prepared on a sub-100 nm range, e.g. by microstructuring processes. A fundamental understanding of the static and dynamic properties of magnetism in the sub-m range is therefore of great importance.

The X-ray magnetic dichroism (X-MCD), i.e. the dependence of the absorption of circularly polarized X-rays on the magnetization of the absorber exhibits at L-edges of transition metals and M-edges in Rare Earth systems values up to 25%. This can serve as a huge magnetic contrast mechanism in combination with a transmission X-ray microscope (TXM) to image magnetic domains providing a lateral resolution down to about 30nm[1]. Major features of this new technique are the inherent chemical specificity to address single elements in a multicomponent system, a high sensitivity allowing to investigate thin films with a thickness corresponding to a few monolayers only and the potential to record the magnetic images within in principal unlimited external magnetic fields, which is in particular essential to characterize the functionality of technological devices[2]. Trial results on thermomagnetically written bits in magneto-optical discs obtained at the XM-1 X-ray microscope at the ALS[3] and the switching behaviour of individual dots in artificially nanostructured multilayered system[4] will be reported. Future perspectives with regard to a time-dependent imaging mode will be outlined. Currently a dedicated magnetic transmission X-ray microscope is being set-up at a helical undulator source at BESSY II.

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Creation of Fundamental Reaction Steps on Single Molecules with a STM-Tip

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The fundamental reaction steps such as dissociation, diffusion, desorption, re-adsorption and association have been performed on single molecules in a controlled manner with a STM tip on Cu(111) surface at 15 K. Selective abstraction of iodine atoms from the single iodo- and diiodo- benzene molecules have been succeeded by using tunneling electrons of 1.5 eV. The necessary threshold voltage to break a single bond inside the molecule was determined by acquiring the I-V tunneling spectrum of the molecule. This selective bond breaking procedure is based on the inherent differences in the bond strengths inside the molecule system and independent on the localised tunnelling through the bond position. The resultant C_6H_5 and C_6H_4 fragments can be further dissociated by using tunneling voltages exceeding 3V. The diffusion processes of the single atoms and molecules on the Cu(111) terrace and at close-packed step-edges were studied by employing the lateral-manipulation technique with the STM tip. The iodine atom can be moved along both [110] and [211] directions while di-iodobenzene prefers to move only along the close-packed row directions on the Cu(111) terrace. Attractive tip-molecule/atom interactions play a key role in this procedure. To observe the molecules' shapes, the STM tip was functionalized by deliberately transferring an iodine atom or a CO molecule into its apex where controlled desorption and re-adsorption processes have been applied. Furthermore, rotation and up-right tilting of the di-iodobenzene molecules can be induced with the STM tip which can be explained by inelastic tunneling and di-polar interaction between the tip and the molecule. The adsorbed molecule positions can be altered at will by applying tip-sample interaction force and the process can be controlled by corresponding tip-height signals. Association between the two molecules can be realized by exciting them with the tunneling electrons where the bond formation process is explained by rotational excitation of the molecules. By choosing suitable combination of manipulation techniques, a whole chemical reaction can be created over the single molecules and as an example, the 'Single-Molecule-Ulmann Reaction' will be presented where bi-phenyl molecules are synthesized individually with the STM tip .

Exchange bias at ferromagnet-antiferromagnet interfaces resolved by Photo-Electron Emission Microscopy

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Antiferromagnetic layers are key-components in advanced magnetic devices, such as magnetization sensors used in hard disks or magnetic random-access memory. The antiferromagnet pins or "exchange biases" a thin ferromagnetic layer, which serves as a magnetic reference to a second, free ferromagnetic layer. Information is stored or magnetic fields are measured via the relative orientation of the two ferromagnetic layers, exploiting the orientation dependent resistance of the element (giant magneto-resistance, GMR effect). Despite of the technological importance of exchange bias, still knowledge is lacking about the mechanism, which couples the two layers, partly because of the inability of traditional techniques to spatially determine the microscopic magnetic structure of the antiferromagnet. We will present results, showing that photo-electron emission microscopy (PEEM) is capable of determining the surface magnetic structure of ferromagnets and antiferromagnets with high spatial resolution (<50 nm). Magnetic dichroism effects at the L edges of the magnetic 3d transition metals, using circularly or linearly polarized soft x-rays provided by a synchrotron source, give rise to a magnetic image contrast. Images acquired with the PEEM2 experiment at the Advanced Light Source, show magnetic contrast on antiferromagnetic $LaFeO_3$, for the first time resolving the magnetic domain structure in an antiferromagnetically ordered thin film [1]. Angle and temperature dependence were used to illuminate the magnetic properties of the material. Magnetic exchange coupling between $LaFeO_3$ and an adjacent, ferromagnetic Co layer results in a complete correlation of their magnetic domain structures. From field dependent measurements a unidirectional anisotropy resulting in a local exchange bias of up to 30 Oe in single domains could be deduced. Apparently, domain correlation and microscopic bias already occur in not field-annealed samples, even though no macroscopic bias was observed [2]. The elemental specificity and the quantitative magnetic sensitivity render PEEM a powerful tool to study magnetic coupling effects in multi-layered thin film samples with high spatial resolution.

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Quasiparticle Energy Bands of NiO in the GW approximation

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We present a first-principle study of the quasiparticle band structure of NiO. The calculations are performed using the spin-polarized GW approximation for the electron self-energy operator with a plane wave basis and ab initio pseudopotentials.

Much efforts have been devoted in the past to understand the electronic structure of this prototype Mott insulator, including the density functional theory and several model calculations. Although the local-spin-density approximation (LSDA) gives satisfactory description to the occupied oxygen-derived states, the observed d-band dispersions are about 25% smaller, and the LSDA band gap is an order of magnitude too small compared to experiment.

There have been two recent studies using GW and model GW approximation on NiO, but the energy gaps obtained do not agree with each other, since the underlying approximations and basis used are different in these two calculations.

Our calculated band gap compares favorably with experiment. The valence band structure agrees with integrated and angle-resolved photoemission experiments in the low binding energy region. Further, we find new features in the electronic structure of nickel oxide which were not known before.

Depth-Profiling by Angular-Dependent X-ray Photoelectron Spectroscopy

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Obtaining depth-profile information from angle-dependent XPS measurements has a long history, and has been a useful method for measuring oxide layer thickness for over twenty years. Recently there is renewed interest in extracting more detailed depth-profile information, driven by

(i) Applications in profiling ultra-thin structures, such as biomaterial surfaces or nitrogen in semiconductor gate-oxides.

(ii) The need for chemical state information to solve industrial problems, information which is rapidly destroyed by alternative sputter-profiling methods.

(iii) The appearance of new XPS instruments from at least three manufacturers, designed for rapid angle-dependent XPS.

We review the problem of converting angle-dependent XPS measurements into a depth-profile a customer can interpret. This is a severely ill-posed inverse problem, intimately linked to the loss of phase information in XPS peak intensity measurement. Elastic scattering of signal photoelectrons is an added complication. By applying a straightforward model of instrument resolution, but in Mellin space rather than the more familiar Fourier space, we derive a good estimate of the depth-resolution possible[1].

To improve on this limit one needs to apply prior information about the structure of the specimen, which in fact one always has in an analytical problem. The variety of information that can be incorporated to solve for different types of specimen has led to at least 20 different algorithms being proposed in the literature, each suitable for one type of specimen or other. To rationalise this diversity we first reviewed the published methods, reducing them to four generic types and identifying the simplest reliable method of each type. These four algorithms have been incorporated into easy-to-use software, refined after use by members of the UK ESCA User Group. This leads to definite recommendations on which method to use for which type of specimen.

Two novel methods will be presented here that address important requirements identified at the end of this exercise,

(a) A new method of calculating film thickness[2], of unprecedented simplicity, and

(b) A method for depth-profiling oxynitrides on silicon, or silicon in oxides on aluminium, using novel inverse-theory to give the best possible depth-resolution.

Photoelectron spectroscopy study on the Si(111)√7x√3-In surface

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The atomic and electronic structures of the √7x√3 phase induced by In adsorption on the Si(111) surface was investigated by angle-resolved photoelectron(ARP) and core-level photoelectron spectroscopy using synchrotron radiation. Recently, among surface reconstructions of the In/Si(111) system, it has been reported that a single domain 4x1 surface has one-dimensional metallic states at room temperature[1] and exhibits phase transition by charge density wave at low temperature[2]. In contrast, the √7x√3 surface, which appears at a little larger coverage than the 4x1-In surface, is expected to show two-dimensional metallic states.

The experiments were done on the newly built high-resolution photoemission beam line BL-1C for surfaces/nanostructures at the Photon Factory.

In 4d and Si 2p core levels were measured with high resolution. The In 4d spectrum of the √7x√3-In surface is fitted by a single component, indicating that the √7x√3-In surface has only a single adsorption site for In. The In 4d spectrum shows a highly asymmetric shape, suggesting a metallic character. The Si 2p spectrum is deconvoluted into two spin-orbit doublets and a satellite peak due to plasmon loss. The satellite suggests that there are free-like electrons in the √7x√3-In surface layer. From analysis of ARP spectra, we have found dispersive surface states together with a metallic surface state that crosses the Fermi level.

These results have revealed that In atoms form a metallic overlayer.

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Multiple Scattering Theory of Photoelectron Angular Distributions and Shape Resonances from Oriented Diatomic Molecules*

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Angular distributions of photoelectrons emitted from fixed-in-space molecules have become an exciting new tool for studying electronic structure and dynamics [1-3]. We here use multiple scattering photoelectron diffraction (MSPD) theory to calculate the final-state wavefunction of the electron leaving the molecule and then subsequently its angular distribution. The effects of non-spherical scattering potentials are included in our formalism through non-diagonal
scattering matrices, which fit directly into a new approach for multiple scattering theory originally based on spherical potentials [4]. When the kinetic energy of the photoelectron is low (E < 50-100 eV), we find that its scattering cannot be adequately represented by spherically-symmetric potentials. In addition, we have considered the effect of the final-state hole on the wavefunction, and found this to be important as well. Different polarizations of the
light are also included. As an example, we calculate the angular distribution of photoelectrons emitted from the K shells of C and O in oriented gas-phase CO molecules, as recently measured by several groups [1-3]. We show that intramolecular scattering and interference are responsible for the experimentally measured patterns. Particularly important are the energies for which shape resonances appear in the continuum, with the angular distributions showing radical changes over such resonances. We find good agreement between our theoretical results and recent experimental measurements [2,3]. This MSPD approach thus represents a more accurate and versatile method for dealing with such angular distributions as compared to prior calculations of such effects [5].

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X-ray photoemission Spectroscopic Study of GaN Surface Chemistry and Electronic Properties during Au Contact Formation

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The wide band gap of GaN (3.6 eV), and its ability to form many alloys with other III-nitride materials make it an excellent material for blue light emitting diodes (LEDs) and blue laser diodes. Efficient devices require metal-nitride contacts with low resistance. A prerequisite for systematically optimizing such contacts is a detailed knowledge of the connection between surface chemistry and the electronic properties of GaN.

It has been shown that HCl treatments can reduce the oxygen and carbon contaminants on the n-GaN surface [1]. KOH reduces the oxide-based contamination layer present on p-GaN [2]. By directly examining such chemically treated n-GaN and p-GaN surfaces with x-ray photoelectron spectroscopy, we have determined the chemical composition and Fermi level pinning for n- and p-type GaN surfaces. The use of a synchrotron light source allows us to tune the incident photon energy and the resulting electron energy for maximum surface sensitivity.

Our results indicate that the KOH treatment reduces the surface barrier height of the p-GaN relative to the HCl-treated samples, with the surface Fermi level of the KOH-treated samples lying ~1.0 eV closer to the valence band maximum (VBM) than the surface Fermi level of the HCl-treated sample. When p-GaN is treated with KOH-based solutions, the ratio of Ga/N decreases while identical samples treated with HCl show an increase in the Ga/N ratio [3]. Samples of n-GaN also show a decreased surface barrier height when treated with HCl.

We will present data on the initial stages of contact formation. After deposition of a sub-monolayer of gold, we observe a new peak in the Ga 3d core level region indicative of a surface chemical reaction with gold. As the gold coverage increases, we see the surface Fermi level shift toward the VBM. With the data collected, we have improved our understanding of contact formation on GaN materials.

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Scanning Tunneling Spectroscopy Analysis with a Triangular Inverse Transfer Matrix and its Application to Reduced SrTiO3 (110) Surface

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A conventional method in scanning tunneling spectroscopy (STS) to deduce sample local density of states (LDOS) from the current-voltage characteristics (I-V) data has been to calculate $(dI/dV)(V/I)$, which corrects for the effect of deformation of tunneling barrier when the bias voltage is comparable to the work functions of tip or sample surfaces. But the conventional method causes an artifact: When the I-V have a local energy gap feature, calculated LDOS tend to show peaks at onsets of tunneling current. We have been introducing an alternative method to deduce LDOS from the I-V data[1]. The I-V data vector, sampled at discrete bias voltage points, is approximated by the LDOS vector multiplied by a triangular transfer matrix M, each row of which is determined by the tip density of states and the barrier profile for the corresponding bias voltage. The LDOS vector is readily calculated from the I-V vector simply by multiplying M^{-1}, which is also a triangular matrix, and site-independent. The triangular inverse transfer matrix M^{-1} has large diagonal and next-to-diagonal elements and slowly decaying elements for the rest part, and converges to the simple differentiation when the bias voltage is small and the deformation of the tunneling barrier is negligible. The density of states of W tips is calculated from the I-V measurement for W tip/ W surface at different tip-to-sample distances. The analysis to calculate LDOS is demonstrated for the reduced SrTiO3 (110) surface where the electronic states show metallic character depending on the annealing condition and sites. In addition, the metallic character is verified by an in situ conductance measurement.

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State and Site Selective Fragmentation of SPF$_3$ Following Inner-Shell Excitation

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A common motivation of much of the research concerning the decay of inner-shell excited and ionised states is the identification of state or site selective relaxation processes. A better understanding of the circumstances under which the high localisation of the core hole formed upon photoabsorption leads to selective bond dissociation in the inner-shell excited molecule is of considerable interest for the development of X-ray wavelength-selective photochemistry .

Results from recent studies of the photofragmentation of thiophosphoryl fluoride (SPF$_3$) will be reported that provide dramatic examples of both state and site selective fragmentation processes. Partial ion yields and ion-pair yields have been obtained using time-of-flight mass spectrometry with multi-coincidence ion detection for SPF$_3$ following phosphorus and sulphur K-shell and L-shell excitation. Inner-shell excitation was performed by absorption of monochromated synchrotron radiation at the Canadian Synchrotron Radiation Facility located at the Synchrotron Radiation Center, U. Wisconsin–Madison.

Examples of highly selective fragmentation processes of SPF$_3$ are found in particular near the phosphorus 2p and sulphur 2p edges. Despite an energy separation between these edges of only approximately 30 eV, certain fragmentation channels are found to dominate at one edge and yet be completely absent at the other edge.

Comparison of the fragmentation processes that occur following K-shell and L-shell excitation indicate that, following excitation of either a phosphorus 1s or sulphur 1s electron, the deep core hole typically relaxes by an Auger cascade, resulting in states of high total charge and leading to extensive molecular fragmentation. Although significant fragmentation is also observed for certain excitations involving phosphorus 2p and sulphur 2p electrons, the total ionisation that occurs is considerably less.

The impact in SPF$_3$ of the location of the inital core hole on the resulting fragmentation processes is illustrated by the observation that, with both K-shell and L-shell excitation, the extent of fragmentation is observed to be greater at the corresponding lower energy phosphorus edge than at the corresponding higher energy sulphur edge.

Ultrafast X-ray Science at the Advanced Light Source*

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An important new area of research in chemistry, condensed matter physics, materials science, and biology is the application of x-ray techniques such as diffraction, EXAFS, XANES, etc. to investigate structural dynamics associated with ultrafast chemical reactions, phase transitions, vibrational energy transfer, and surface dynamics. Such processes are driven by atomic motion and rearrangement occurring on the fundamental time scale of a single vibrational period (~100 fs). While third generation synchrotrons are powerful tools for probing the time-average structure of matter, their time resolution is limited to >30 ps, as determined by the duration of the stored electron bunches. We have recently demonstrated the generation of femtosecond synchrotron pulses from the Advanced Light Source using a novel laser slicing technique[1,2]. Femtosecond laser pulses are used to create femtosecond time structure on a long electron bunch via energy modulation and subsequent spatial separation of an ultrashort slice of electrons. Femtosecond x-rays are then generated from the ultrashort electron slice. Modulation of the electron energy is accomplished by co-propagating a femtosecond laser pulse with the stored electron bunch through a resonantly tuned wiggler. The laser field accelerates the underlying electrons by an amount that is several times larger than the rms beam energy spread. Modulated electrons are then spatially separated from the main electron bunch (in a dispersive bend of the ring) by a transverse distance that is several times the rms transverse size of the electron beam. By imaging the synchrotron radiation from the displaced beam slice to the experimental area, we are able to separate out the femtosecond pulses originating from the offset electrons. Synchrotron pulses of ~300 fs duration are directly measured by cross-correlating the visible radiation from a bend magnet with a femtosecond laser pulse. A new bend-magnet beamline at the ALS is now being commissioned, and will generate 100 fs x-ray pulses in the 1 to 10 keV range with an average flux of $\sim 10^5$ ph/s/0.1%BW and an average brightness of $\sim 10^8$ ph/s/mm^2/mrad^2/0.1%BW. A small-gap undulator beamline is being proposed for the ALS, and this beamline is designed to provide 200 fs x-ray pulses in the 1 to 10 keV range with an average flux of $\sim 10^8$ ph/s/0.1%BW and an average brightness of $\sim 10^{12}$ ph/s/mm^2/mrad^2/0.1%BW. The capabilities of these beamlines will open new research areas in ultrafast structural dynamics in condensed matter.

Resonant Soft X-ray Raman Spectra of Ni and Co Oxides at Metal 3p Threshold

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Resonant x-ray Raman spectra of NiO (100) and CoO (100) single crystals, measured at corresponding transition metal 3p thresholds, are discussed in terms of d-d excitations. In contrast to measurements at 2p thresholds, transitions to low-lying excited crystal-field-split states are clearly resolved. At the same time, the observation of "magnon" states with the energy losses under 0.5 eV is hampered due to the presence of an intense elastic peak in these spectra. The data are compared with the results of Anderson impurity model calculations and optical absorption and low-energy electron-energy-loss measurements.

Nature of the Sn/Ge(111) phase transition: Charge density waves or dynamical fluctuations?*

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Critical phenomena are a fascinating area of current research in solid state physics. The complex phenomenology of the phase transitions is frequently related to a rich mixture of electronic and structural effects which can be better analyzed in a low-dimensional playground. Recently, Carpinelli et al. [1] have reported a temperature-driven phase transition for a Pb or Sn layer deposited on Ge(111). At room temperature, 1/3 of monolayer of Pb or Sn atoms occupy T4 sites of the Ge(111) surface, giving rise to a $\sqrt{3}\times\sqrt{3}R30^{\circ}$ surface periodicity. As temperature decreases below 250 K, a 3x3 surface phase appears. The 3x3 ground state was described as the stabilization of a charge density wave (CDW) in the Pb layer, driven by electron-phonon coupling in the two dimensional Fermi surface. A similar behavior has been observed for Sn/Ge(111) interfaces. In a wide range of low dimensional metals, CDWs are stabilized at low temperatures, however, Pb and Sn deposited on Ge(111) are the first examples of surface charge density waves. In a CDW state, energy gaps open in flat areas of the Fermi Surface (FS) joined by a wave vector ``nesting vector'' equal to twice the Fermi momentum k_F. A structural study performed by the same group found no significant rippling in the Sn layer, and attributed the 3x3 phase to lateral atomic displacements in the first Ge layer. In addition, Melechko et al [2] and Weitering et al [3], have recently observed a significant number of defects in the Sn-(V3xV3)R30° phase. They found that defects act as seeds for the nucleation of the (3x3) phase and that the temperature of the phase transition depends on the defect concentration. Following these ideas, a defect-mediated CDW may be established at the surface and it could provoke the phase transition. This scenario has been recently questioned in several aspects by LURE-Madrid group [4,5]. First, the experimental Fermi surface exhibits no significant nesting, a crucial point in the theoretical model proposed in Ref. 1. Second, valence-band photoemission results do not support that electron correlation plays a major role in 3x3 phases. Third, in disagreement with theoretical calculations of ref. 1, the surface valence bands are split in both phases. Moreover, core-level photoemission for Sn/Ge(111) indicates the existence of two kinds of Sn atoms in the room and low temperature phases. All these experimental results can be easily rationalized assuming a corrugated Sn or Pb layer which excludes the stabilization of a CDW. Our recent Surface X-ray Diffraction results [5] confirm the existence of this effective vertical adsorbate layer distortion. We conclude that the origin of this reversible temperature transition from the $\sqrt{3}\times\sqrt{3}R30^{\circ}$ phase to the 3x3 phase is not a CDW. Both phases have a strong rippling of the Sn (Pb) layer ($\approx$ 0.4 Å) with two Sn (or Pb) inequivalent adatoms. At room temperature the overlayer atoms are fluctuating between these two distinctive sites and at low temperature the fluctuation is frozen. *This work has been supported by the CICYT and the European

Development of a High-Speed One-Dimensional Detector for Electron and Other Spectroscopies*

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The continued development of brighter synchrotron radiation and other radiation sources throughout the world has resulted in increasingly more intense excitation sources for use in photoemission and related Auger and x-ray emission experiments. The development of the detectors used in these experiments has unfortunately not kept pace with these advances and consequently many experiments today are limited in data acquisition rate and/or energy resolution by the capabilities of the detector. This is particularly true in electron spectroscopy at third-generation synchrotron radiation sources, but it also affects work with the most intense laboratory-based sources such as rotating anode x-ray tubes. Even standard XPS systems can exhibit significant non-linearities in counting that can affect quantitative analyses of spectra [1]. As a first step toward bridging this "detector gap", we have developed a one-dimensional high-speed detector system with a spatial resolution of 75 microns over 768 parallel channels. Each channel is capable of greater than 1 MHz counting frequency, resulting in about 1 GHz maximum overall counting rate and a high degree of linearity over the full range from 0 to 1 GHz. The resolution is better than that available in any current system, and the counting rate represents a significant step forward, being ~50-1000x greater than that of existing detectors. The detector is based on a microchannel plate multiplier, followed by individual collector strips connected to in situ application-specific integrated circuits for preamplification and counting. It has been specifically designed for photoemission experiments performed with a hemispherical analyzer. However the detector is inherently capable of counting other particles, including visible, UV, or x-ray photons and ions, and should therefore be of general use in particle counting experiments requiring a large dynamic range and one-dimensional spatial resolution. We will present the design of the detector, the testing procedures and results, and photoelectron spectra acquired with a first prototype installed in a Scienta ES200 spectrometer.

Electron-Ion Coincidence Spectroscopy Studies of Ion Desorption Induced by Core-Electron Transitions of Surfaces

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Energy-selected electron ion coincidence (EICO) spectroscopy combined with synchrotron radiation is a novel tool for photoelectron spectroscopy of specific sites responsible for ion desorption [1]. We have developed an EICO apparatus, which consists of a cylindrical mirror electron energy analyzer and a time-of-flight ion mass spectrometer [1-3]. In a study of condensed H_2O using photoelectron photoion coincidence (PEPICO) spectroscopy, the peak position of Oxygen 1s photoelectron was observed to be shifted by 0.7 eV from that in PEPICO yield spectrum. This result was attributed to the difference of chemical environment between the surface H_2O responsible for H^+ desorption and the bulk H_2O. A PEPICO study of a fluorine-saturated Si(111) surface showed that Si 2p ionization at SiF, SiF_2, and SiF_3 sites are responsible for F^+ desorption [4]. The EICO spectroscopy is powerful also for elucidating mechanism of ion desorption induced by electron transitions, because it provides ion mass spectra for the ion desorption channels related to the selected electron transitions [1-3]. A study of condensed H_2O using Auger electron photoion coincidence (AEPICO) spectroscopy showed that H^+ desorption is stimulated by O KVV Auger processes leaving two-hole states. The H^+ desorption probability is found to depend on the bonding character of the orbitals where holes are created and on the effective hole-hole Coulomb repulsion. AEPICO investigations of H^+ desorption induced by resonant core-electron excitations of condensed H_2O clearly showed that one-electron-one-core-hole state or one-electron-two-valence-hole states are responsible for the H^+ desorption mechanism.

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The sudden Approximation in Photoemission: When is it valid?

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We define the sudden approximation (SA) as the bulk one-electron spectral function augmented with dipole matrix elements. This approximation is exact in the high energy limit for isolated systems like atoms and molecules. For solids, where the electrons come from a surface region and the mean free path is an important feature, SA is never valid, not even at high energies. Here the correct high energy limit is a convolution of the sudden approximation and the loss function (SA*LF). SA is particularly valuable when we only look for peak positions such as quasi-particle energies (e g for bandstructure mapping). It may be argued that also quasi-particle lineshapes are well represented. When it comes to broader spectral properties, which are important for e g strongly correlated systems, SA can no longer be relied on. For core level photoemission from weakly correlated systems like metals and valence semiconductors SA*LF correctly describes the satellite intensities only in the keV region, while the asymmetric quasi-particle line shape (in metals) is given correctly by SA already at low energies [1]. For localized strongly correlated systems SA is reached rather quickly, say at 10-20 eV above threshold [2]. We also discuss the often used one-step model for photoemission [1], and strongly correlated layered systems [3]. The presentation partly builds on a recent review article [4].

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Ultrafast time-resolved x-ray measurements of polaron dynamics of charge-ordered Nd$_{1/2}$Sr$_{1/2}$MnO$_3$

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We investigate the role of the Jahn-Teller (JT) interaction in Nd$_{1/2}$Sr$_{1/2}$MnO$_3$ by time-resolved x-ray measurements of the polaron dynamics. The formation and relaxation of the polarons, induced by photo-carriers, are clearly observed in picosecond dynamics of the diffuse x-ray scattering. We monitor how the lattice structure evolves after the material is irradiated with 150-fs, 800-nm laser pulses. The pump-laser wavelength overlaps with the broad Mn3+ to Mn4+ charge-transfer transition band. The lattice dynamics is probed with the time-resolved x-ray Bragg diffraction from the orthorhombic Pbnm (112) plane of a single crystal Nd$_{1/2}$Sr$_{1/2}$MnO$_3$. The experiment was performed at beamline 7.3.3 of the Advanced Light Source. Strong diffuse scattering, indicative of a large lattice distortion, is observed to develop over $\sim$ 30 ps and to relax in 300 ps. The observed laser-induced modification of the x-ray Bragg diffraction is a direct result of the strong coupling between the JT lattice distortion and the charge-transfer transition. Impulsive (faster than the lattice can respond) charge-transfer from ions to ions would create the JT lattice distortion. We model the observed data assuming that the charge-transfer transition creates the anisotropic JT distortions. Relative to the lattice plane, which corresponds to (101) of the cubic perovskite, these distortions amount to longitudinal expansion and transverse compression. The longitudinal and transverse strain associated with the JT distortions propagate into the crystal with the relevant speed of sound. From the calculation, we estimate that the JT distortions decay in $\sim$ 50 ps and the JT interaction energy is $\sim$ 1 eV independent of temperature.

Atomic Scale Magnetic Mmaging of Ultrathin Films

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Magnetic nanostructures are promising candidates for ultra-high density data storage media. Due to lack of high resolution magnetic imaging techniques their properties have, however, mainly been investigated using spatially averaging techniques. Spin-polarized scanning tunneling microscopy/spectroscopy (SP-STM/STS) using magnetic probe tips has long been considered as a promising tool in order to study magnetic properties down to the atomic scale. In the past we have focused our effort on the Gd(0001) surface which exhibits an exchange-split surface state [1] and can therefore be regarded as a model system for SP-STS. We showed that SP-STS allows the separation and correlation of topographic, electronic and magnetic properties within a single measurement [2].

Recently, we have performed experiments on self-organized Fe-nanowires and antiferromagnetic Mn films. The thickness of the nanowires amounts to two atomic layers only. Based on a detailed investigation of the spin-resolved electronic structure we could clearly observe the magnetic domain structure of the nanowires. It is governed by a dipolar antiferromagnetic coupling of adjacent wires which is mediated by the stray field. Our images allow the evaluation of the influence of structural defects such as, e.g., non-uniform width and separation of the wires.

As early as 1988 the 2D antiferromagnetic structure of a monolayer Mn film on non-magnetic substrates has been theoretically proposed [3]. Only now we could proof this proposal by atomic-resolution SP-STM. The SP-STM experiments are explained on the basis of ab-initio electronic structure calculations using the full-potential linearized augmented plane wave (FLAPW) method.

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Direct Photoemission from Image Potential States of Epitaxial Ag (111) Films on WSe$_2$ (0001)

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Ag grows on the van der Waals plane of WSe2 azimuthally ordered islands exposing a clean (111) surface to vacuum. Accordingly a LEED pattern of Ag (111) is superimposed on the WSe2 pattern and the Shockley type surface state S1 of clean Ag (111) is observed in photoemission with 21 eV in normal emission. At the Schottky barrier a nonequilibrium surface photo voltage is generated. Excitation with photon energies in the range of 3.8-5 eV electron emission below the threshold (as determined by the macroscopic secondary cutoff) is observed which is attributed to a resonant excitation of electrons originating from S1 into image states n=1 and n=2 of the Ag (111) surface of the islands. An emission due to 2PPE is ruled out. Tentatively we explain the subthreshold emission due to the formation of a triple junction at the Schottky barrier Ag/WSe2 interface. Electrons resonantly excited to image states n=1 and n=2 above a Ag (111) oriented island may escape at the edge of the island into vacuum. #

Resonant Photoemission of ICE epitaxially grown on Pt(111)

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We have studied resonant photoemission around the O K edge of ICE epitaxially grown on Pt(111). The resonant processes probes the intermediate states, and dynamical properties on the time scale of the core-hole lifetime can be extracted.

The measurements were performed using the surface end station at undulator beam line I511 at MAX-lab (Sweden). The end station is equipped with a spherical electron spectrometer rotatable around the incoming light axis. This capability allows us to measure XPS at normal emission using two different geometries; one with the E vector in the plane of the sample surface ("Auger" geometry) and the other with the E-vector normal to it ("photoemission" geometry). Since the cross-section of photoemission(dipole) channels in the "Auger" geometry is surpressed, one can distinguish the Auger-like processes from the photoemission-like.

A series of XPS spectra were measured as a function of photon energy at both geometries. Each spectrum covers the valence/inner-valence photoemission peaks and the oxygen Auger peaks. Two dimensional XPS spectra were plotted as a function of photon energy and electron energy for each geometry. Comparing them, the assignment of the resonant processes was clarified.

The XAS spectrum shows a preedge peak at 535 eV, a second peak at around 536.5 eV followed by a transition to a continuum of states (maxima at around 540.5eV). At the preedge, the photoemission peaks (1 hole final state) in the XPS spectra shows a resonant Raman behavior, i.e. surpressed below the edge and much enhanced on the edge. Also spectator Auger (1 hole 1 particle) peaks can be seen. The second edge is the onset of both pure Auger-like (constant kinetic energy) and photoemission-like (constant binding energy) spectral features. A post collision interaction-like process is also seen for the main oxygen Auger line. In the continuum of states region, both pure Auger-like and resonant Raman processes are manifested.

In the poster we will discuss the nature of the resonant processes involved, and extract information about the intermediate states in terms of localization/lifetime. Detailed plots will be presented with assignation of the processes/final states together with the conclusions that can be drawn from them.

X-ray emission and resonant inelastic scattering - Present and future.

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The third generation synchrotron radiation sources have made soft X-ray spectroscopy become a new tool to be applied towards a better understanding of complex new materials, processes and technologies. The photon-in photon-out technique offers some unique and valuable advantages. Most of these are derived from the fact that photons are tunable in energy, carry polarization, have a large penetration depth, are insensitive to electric and magnetic fields, and exhibit coherent properties. The most important assets include element and chemical-state specificity, probing of the true bulk properties and the ability to study buried interfaces with sub-monolayer sensitivity. Also, it allows the study of electro-chemical processes at the solid liquid interface or biological samples in their natural wet state.

An account is presented for recent developments and future prospects in resonant soft X-ray emission studies of materials and surfaces, and examples include studies of solids, interfaces, gases and liquids.

Plasmon energy shift in Porous Silicon measured by X-Ray Photoelectron Spectroscopy (XPS)

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In order to provide experimental support for quantum confinement models [1,2] describing electronic effects in porous silicon (p-Si), the Si2s and Si 2p plasmon losses have been studied by X-Ray Photoelectron Spectroscopy (XPS). The p-Si surface was cleaned by an ethanol solution containing HF, thus avoiding possible damages induced by any subsequent cleaning by ion sputtering. The p-Si plasmon energy was found at ~ 19 eV. This value, ~ 1.6 eV higher than that of bulk Si (17.4 eV), as measured on the cleaned Si substrate as a reference, is quite reproducible on all the samples studied in this experiment. The magnitude of this blue shift suggests possible quantum confinement effects that could be ascribed to the p-Si nanostructures; however, the influence of spurious Si-O-H-like compounds on the various internal and external surfaces of the material needs further investigation.

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A HIGH-RESOLUTION NEXAFS STUDY OF AN AZIMUTHALLY ORIENTED MOLECULE: BITHIOPHENE ON Ni(110)-S AND Cu(110)-O SURFACES

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Sulfur reconstructed Ni(110)p(4x1) and oxygen reconstructed Cu(110)(2x1) single crystal surfaces have been used as templates for the adsorption of thin films of bithiophene. Bithiophene, being the smallest of the oligothiophenes, is a useful experimental model for controlled UHV studies, while still exhibiting the important properties of the larger, in device technology relevant oligomers. Both templated substrates induce the molecules in the monolayer to adopt a preferred azimuthal orientation, as evidenced by a variety of techniques. Here we focus on the carbon K and sulfur L2,3 NEXAFS and their ability to determine the molecular geometry. High-resolution NEXAFS of bithiophene multilayers are markedly different to thiophene - in particular the carbon K spectra are clearly a superposition arising from the inequivalent carbon sites. On both surfaces the NEXAFS data unambiguously demonstrate that the molecules are considerably tilted with respect to the surface. Th azimuthal ordering leads to significant differences in the angular variation of NEXAFS in the two principal surface azimuths. This must be taken into consideration when determining the molecular tilt. The molecular orientation thus determined by NEXAFS will be discussed in the light of recent HREELS [1] and ARUPS [2] results.

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Differential Photoelectron Holography: A New Approach to the Forward-Scattering Problem

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We propose a new method to improve the imaging ability of photoelectron holography (PH) by simply using "difference" holograms over multiple wave numbers. Len et al. have analyzed both experimental and theoretical large data sets for W(110) and demonstrated that the images of atoms lying under a photoelectron emitter are well reconstructed by all the five principal algorithms so far proposed, while only limited success could be achieved for imaging the atoms in the forward-scattering (FS) directions owing to strongly anisotropic atomic scattering amplitudes [1]. This makes it more difficult to apply PH to many systems where FS may play a critical role, such as bulk crystals, epitaxial films, buried interfaces, as well as some adsorbed and reconstructed surfaces that include scattering atoms between the emitter and the detector. A prior method in which scattering-factor anisotropy is corrected for [2] has the limitation that it cannot be applied to compound materials, where an atom-specific probe like PH would play an important role. To overcome this difficulty, we propose the idea of differential holography in which strong FS peaks can be effectively removed by subtracting two holograms with slightly different wave numbers, while holographic interference fringes that are very sensitive to the change in the wave number will survive this subtraction. We have tested this method by multiple-scattering simulations of photoelectron holograms from Cu(100): we find that differential PH is successful in depressing strong FS effects so that atoms in forward, side and backward directions as viewed by emitters can be imaged if appropriate experimental conditions are chosen.

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Direct observation of depth profile of magnetic moment by magnetic circular dichroism

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The magnetic properties at the interface between Fe and Cr wedge layers are investigated with a new depth-resolved soft x-ray photoemission spectroscopy (SXPS)[1], combined with magnetic circular dichroism (MCD). The layers of Fe (10 A)/ Cr (50 A wedge-shaped) are grown on a periodic multilayer (B $_4$ C(22.5A)/W(17.1 A)) $_{40}$, which provides the strong standing wave effects of ~40 % at photon energy hv = 825 eV. The unique angular dependence of photoelectron intensity of Fe and Cr has been observed at each different Cr wedge thickness and show excellent agreement with the theoretical calculation. To maximize the enhancement and contrast of standing wave effect inside of sample, the sample position is tuned to the Bragg angle position, at which the MCD measurement with SXPS along the different thickness of Cr wedge layer provides the depth profile of the magnetic moment of Fe and Cr. A strong antiparallel coupling across the interface of Cr magnetic moment is clearly resolved while the apparent reduction of Fe magnetic moment is observed near the interface. This observation is consistent with the other works on the same system [2] and even describes how the magnetic moment behaves inside of the sample from the top surface to the interface in one single sample preparation. In this experiment, a new depth-resolved SXPS has been successfully implemented to magnetic multilayer system and prove to be powerful technique to study the buried interface of magnetic system, as proposed by our former work [1].

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Depth-Resolved Photoemission Spectroscopy From Surface and Buried Layers with Soft X-Ray Standing Waves

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We have demonstrated a new type of depth-resolved soft x-ray photoemission spectroscopy in which depth sensitivity is provided by means of a periodic multilayer that generates sizeable standing waves above its surface. It is observed that the photoelectron intensities of each element in a complex sample are strongly modulated when the x-ray incidence is scanned over the Bragg condition, and that these modulations show unique behavior depending on the particular position in the sample that each element and/or chemical state is situated, including elements in the first couple of buried layers of the multilayer extending up to about 40 Å inward from the surface The depth-dependent contributions to each intensity can be obtained as the standing wave scans through the buried layers and the interfaces between them. Other future possibilities are adding measurements of valence SXPS spectra to permit deriving depth-dependent densities of states, or adding linear or circular dichroism measurements, or spin resolution of the outgoing electron, to much enhance what can be learned in this way about magnetic multilayer structures (as done already in XMCD10). Going to higher photon energies and/or using fluorescent x-ray detection will also make the technique more bulk sensitive and capable of probing deeper interfaces. Depth-resolved photoemission with soft x-ray standing waves is this a very promising tool for studying surface and interface electronic and magnetic properties.

Electronic structure and magnetism of 3d metals and alloys on GaAs

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The 3d transition metals and alloys exist in a variety of crystallographic and magnetic phases. Thin-film growth of these materials on semiconductor substrates can drive the films into specific crystalline structures. These structures may be in a thermodynamically stable phase, a known high-pressure or high-temperature phase, or even a phase not previously observed. They greatly increase the variety of magnetic materials by essentially making °*new°± materials from °*old°± elements. In this talk we report our recent work on the electronic structure and magnetism of Ni/GaAs(001), FeMn/GaAs(001) and Co/Mn/Co/GaAs(001). It is found that Ni shows a negative K1 magnetic cubic anisotropy, FeMn shows a ferromagnetic to antiferromagnetic transition as a function of film thickness, and Co/Mn/Co/GaAs(001) shows a °*negative°± remanence in the magnetic hysteresis loops. All these new and interesting results will be explained and discussed.

Surface Reconstruction of (2x1)O/Cu[110] : A Complete Structural Characterization by Scanned-Energy and Scanned-Angle Photoelectron Diffraction

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The chemisorption of oxygen on Cu(110) is well known to give rise to a reconstruction of the surface Cu atoms. In particular, the oxygen-induced structural change of the Cu atoms in the uppermost layers has been studied exhaustively over the last couple of decades, and is now generally believed to result in a missing-row structure. However, the position of oxygen and the interlayer spacing between the topmost surface layers of Cu is not still known with any certainty. Even though many different experimental techniques have been used to investigate this simple, yet intriguing, system, the results of different measurements have often proven to be inconsistent with one another.

In this study, we have determined the several structural parameters that are under debate for this system with two well-known and complementary surface structure probes: scanned-energy photoelectron diffraction using synchrotron radiation (also called angle-resolved photoemission fine structure or ARPEFS) and scanned-angle photoelectron diffraction using laboratory x-ray excitation (also known as x-ray photoelectron diffraction or XPD). The ARPEFS measurements have been performed at Beamline 9.3.2 of the Advanced Light Source (ALS) using the Applied Materials Chamber. The XPD measurements have been carried out with a laboratory x-ray photoelectron spectrometer (Hewlett Packard HP5950A) equipped with a special automated goniometer and a non-monochromatized Al Ka x-ray source. In both sets of experiments, the oxygen 1s intensity has been monitored, thus directly probing the local atomic structure around the adsorbed atom. The ARPEFS data was analyzed using a multiple scattering program developed by Chen et al., with structural parameters being optimized via R factors. It was found that having both the ARPEFS and XPD results as cross checks on one another was crucial to arriving at the correct structure, with both sets of data exhibiting distinct diffraction features of different types: oscillatory modulations with energy of ~±15% in ARPEFS, and forward scattering features of ~15-20% in amplitude in XPD. For the ARPEFS analysis, it was also found that photoelectrons with very low take-off angles with respect to the surface (< 12°) are subject to highly preferential scattering events along the emitter-detector direction, and that correctly including enough scatterers along such directions is crucial for accurately simulating the experimental data with multiple-scattering theory. The final structural conclusions of this analysis will be presented.

Magnetic Imaging of NiO/Ag(001) Thin Film using PhotoEmission Electron Microscope

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Technical developments of X-ray Fluorescence Holography

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With recent technical developments, such as the use of optimized source parameters, improvements of the detector system and data evaluation procedures, x-ray fluorescence holography (XFH) is now a technique of sufficient maturity for first applications. From a practical point of view, this method can be situated somewhere between EXAFS and standard x-ray diffraction techniques. EXAFS provides high resolution atomic distances with ordered and disordered samples, but lacks true 3D information and the possibility of distinguishing different atomic shells as we go far from the absorbing atoms. X-ray diffraction on sufficiently large and well ordered crystals provides long range order parameters but lacks direct phase information and short range order information. XFH by contrast works with lower quality and smaller crystals and with systems without translational order but with orientational order, provides direct short range order information, but lacks information on distant atoms beyond the first ~100 atoms. We will discuss recent experimental results obtained at the European Synchrotron Radiation Facility, and new evaluation procedures on different systems and show some examples of the capabilities of this method.

Localization vs. delocalization in Auger resonant Raman scattering at the Cu 2p edges

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Resonant photoemission is a powerful tool for electronic structure studies, e.g. of lanthanides, actinides and 3d transition metals[1]. In recent years the concept of resonant photoemission has been much discussed and much focus has been on the localization vs delocalization of the core-excited intermediate state as a prerequisite for Auger resonant Raman scattering and the channel interference with the direct photoemission channel, leading to the photoemission resonance. Recently unambiguous evidence of channel interference between the Auger resonant Raman and the direct photoemission channels has been presented for the 3d transition metal Ni[2]. The occurence of this resonance has been controversial for a long time, as the core-excited intermediate state in the 3d metals were thought to be not localized enough to allow the resonance process to occure.

In the present contribution, we investigated coherent Auger resonant Raman scattering into the continuum resonances in Cu. Polarization dependent resonant photoemission on the Cu 2p-edges has been performed, indicating dominating Auger resonant Raman scattering. At photon energies 4.2 eV and 7.7 eV above threshold, significant deviations from constant kinetic energy of the normal Auger are found. In a simple scattering calculation these deviations are identified as signatures of Auger resonant Raman scattering at van Hove singularities at the $L_{(1)}$ and $X_{(1)}$ points of the Cu fcc bandstructure at 4.2~eV and 7.7~eV above E_{Fermi}. Opposite to general expectation, coherent Auger resonant Raman scattering into the highly delocalized continuum states of the Cu metal occures to a large fraction. The results provide a link between the Auger resonant Raman scattering description near threshold and the normal Auger decay for continuum-excitation, largely independent of the degree of localization in a system. Both threshold and continuum excitation are found to be coherent Auger resonant Raman scattering. In this light, Auger resonant Raman scattering into a featureless (flat) continuum may still be described in the simple picture of normal Auger decay, as for the special case of a flat continuum the two descriptions are phenomenologically indistinguishable. In particular, these results suggest that the occurence of resonant photoemission is largely independent of the electron localization.

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Fermiology of metals from 1 to 6 dimensions

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The least bound, or Fermi, electrons determine the properties of metals. With momenta that are confined to well-defined surfaces in k-space, and excitations down to zero energy, the electrons are coupled to perturbations with a variety of length and energy scales. Since the degree of this coupling depends strongly on the particular shape of the Fermi surface, understanding many interesting phenomena in metals requires detailed measurements of the Fermi surface topology ("Fermiology").

In this talk I will review recent results for visualization of the Fermi surface and its underlying bands. The experiments were performed at the high-resolution photoemission endstation at beamline 7.0 of the Advanced Light Source. We studied the underlying electronic structure behind a number of phenomena exhibited by metals of different dimensionality: a Peierls transition in 1-dimensional quantum wires [1], magnetic properties of 2-dimensional quantum wells [2], spin-density wave formation in bulk antiferromagnetic Cr [3], and unusual properties of bulk quasicrystals [4] (whose atomic arrangements are projections from 5 and 6-dimensional spaces!).

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Surface Antiferromagnetism of NiO studied by Photoemission Micrsocopy*

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Surfaces of NiO single crystals were studied by polarization dependent soft x-ray absorption. By monitoring the absorption via the total yield of electrons in a photoemission microscope, spatially resolved information is obtained. By tuning the photon energy to the 2p absorption threshold, linear dichroism can be employed to reveal different orientations of the antiferromagnetic vector (i.e. the difference of the two sublattice magnetizations) in antiferromagnetic (AF) domains close to the surface. Using s-polarized light (electric field within the surface) reveals so-called T domains which are associated with antiferromagnetic stacking in (111) directions. The polarization dependence is investigated by azimuthal rotation of the sample as well as by using p-polarized light. One finds a sign change of the contrast for every 90° of rotation, as expected for the T domains with large in plane components of magnetic moments. The AF contrast disappears reversibly on heating to the surface Néel temperature, which agrees within experimental accuracy with the bulk Néel temperature. The domain pattern which re-appears on cooling down is unchanged. Also, the domains are not affected by surface topography. This suggests that the domain topology is governed by defects, which lead to nucleation of domains at specific sites.

Surface structure of the lithiated graphite thin film by x-ray photoelectron diffraction.

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The surface structure of lithiated graphite (Li_xC_6) thin film was identified by x-ray photoelectron diffraction (XPD) measurement on Li 1s and C 1s core levels. In order to do in-situ XPD measurement, Li_xC_6 thin films have been grown on the highly oriented pyloric graphite (HOPG) basal plane in ultra-high vacuum (UHV) chamber by evaporation of lithium from lithium-aluminum alloy source. The fully lithium intercalated structure into graphite was obtained around 400K while metal lithium overlayer formation is observed under 270K of HOPG. The experimental XPD spectra on the lithium intercalated over layers are quite good agreement with calculations by multiple-scattering of photoelectron diffraction based on Rehr-Albers separable representation on the model surface of HOPG and LiC_6 . Li 1s XPD spectra show that the Li_xC_6 thin film has LiC_6 structure and the top surface layer is carbon terminated surface on LiC_6.