

**CONTRIBUTED POSTERS**  
**WEDNESDAY, JULY 25**



# **INTERFACES**



# C<sub>70</sub> adsorbed on Cu(111): interaction and molecular orientation

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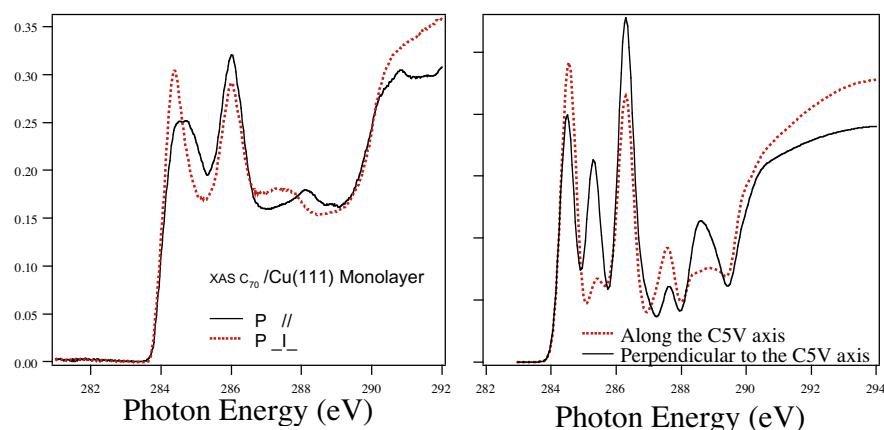
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## ABSTRACT

Although there have been a huge number of studies about the interaction of C<sub>60</sub> with metal surfaces, so far such a kind of investigations are not available for the parent molecule C<sub>70</sub>. By exploiting the unique capability of the ALOISA beamline to change the angle between the linear polarization vector of the photons and the sample surface, without changing any other geometrical parameter, we have investigated the interaction of C<sub>70</sub> with the Cu(111) surface using x-ray photoemission spectroscopy (XPS) and near-edge x-ray absorption fine structure spectroscopy (NEXAFS).

The data point to a net charge transfer from the Cu substrate to the C<sub>70</sub> molecules directly bonded to the Cu atoms, providing a metallic character for a single layer of C<sub>70</sub> (monolayer) adsorbed on this surface. The charge state and metallicity of the C<sub>70</sub> monolayer have been further tailored by adding Na atoms, showing that is possible to fill continuously the LUMO derived states with electrons. This behavior is at variance with the behavior observed in bulk C<sub>70</sub> compounds, where no stable metallic phases form by Na intercalation. Finally, we observe a strong light polarization dependence of the NEXAFS spectra. The comparison between the experimental data and density-functional calculations of the expected contribution to the NEXAFS spectrum of the five inequivalent carbon atoms in the C<sub>70</sub> cage, suggests the molecules mainly oriented with the C<sub>5V</sub> axis almost perpendicular to the Cu surface.



**Figure:** Experimental (left) and calculated (right) NEXAFS spectra of C<sub>70</sub>.

# BURIED INTERFACES OF HEAT-LOADED Mo/Si MULTILAYERS STUDIED BY SOFT-X-RAY EMISSION SPECTROSCOPY

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Soft-x-ray emission (SXE) spectroscopy is a useful tool to study chemical bonding of buried interfaces. Using this method, we have shown that  $\text{Mo}_3\text{Si}$  is formed at the interfaces of as-deposited Mo/Si multilayer (ML) coatings [1]. A Mo/Si ML coating is very useful for its high reflectance at normal incidence for soft x-rays. By using it, novel optical systems, such as soft-x-ray lithography and microscopes, have been developed. For the use as a first mirror in SR beamlines or cavities for soft-x-ray lasers the thermal stability is a serious problem, because the ML structure is broken by the heat load of the intense light. It is important to study this mechanism for the development of thermally stable ML coatings. In this study we measured Si  $L_{2,3}$  SXE spectra for annealed Mo/Si ML coatings.

Mo/Si ML samples were made by a magnetron sputtering system. Annealing was performed under various temperatures and times. Before and after annealing we measured x-ray diffraction and soft-x-ray reflectivity for the samples. SXE spectra were measured at beamline BL-12A of the Photon Factory, KEK. We also measured SXE spectra of some bulk compounds as reference data.

The Si  $L_{2,3}$  SXE spectra of some samples are shown in Fig. 1. The spectrum of the not-annealed sample resembles that of amorphous Si ( $a\text{-Si}$ ) because most part of the Si layers is amorphous. The spectrum of the 400 °C – 5 hours annealed sample is different from that of the not-annealed one. The spectrum of the 10 hours one is more different. Comparison with that of  $\text{MoSi}_2$  suggests that this change is caused by formation of  $\text{MoSi}_2$  at the interfaces on annealing.

From the spectra, we are going to estimate the thickness of the  $\text{MoSi}_2$  interlayers and compare it with the results of the x-ray diffraction and reflectivity measurements.

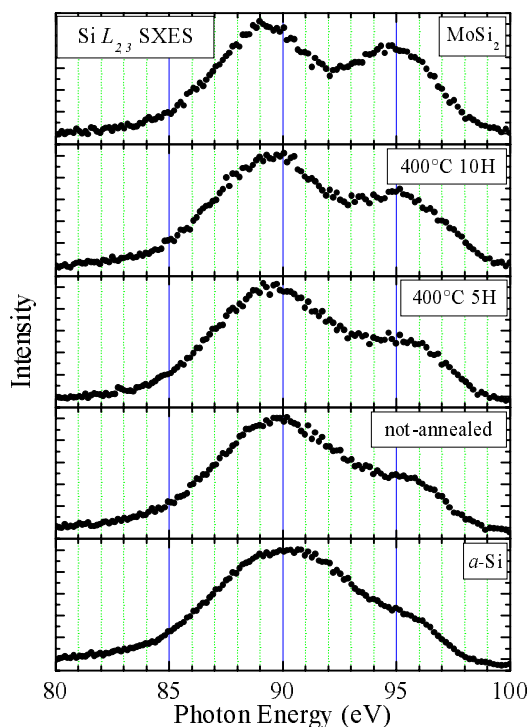


Figure 1: Si  $L_{2,3}$  SXE spectra of  $\text{MoSi}_2$ , 400°C-10 hours annealed ML coating, 400 °C-5 hours annealed, not-annealed and  $a\text{-Si}$ .

## Reference

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# Si $L_{2,3}$ EMISSION SPECTRA FROM THE INTERFACES IN ANTIFERROMAGNETICALLY COUPLED Fe/Si MULTILAYERS

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Fe/Si multilayers are known to exhibit remarkable magnetic coupling between the Fe layers. The origin of the interlayer coupling has been widely investigated, but the proposed models are quite controversial. The most possible reason is that severe interdiffusion occurs at Fe/Si interfaces during sample preparation. Kitakami *et al.* [1] studied the interlayer coupling for a series of Fe/Fe<sub>1-x</sub>Si<sub>x</sub> (0.4 < x < 1.0) multilayers, and suggested the quantum interference model from the results that the antiferromagnetic coupling appeared above x = 0.5 with the nonmagnetic and highly resistive spacer layer, while the layer was ferromagnetic below x = 0.5. Moreover, the coupling strength was enhanced dramatically with increasing x for 0.5 < x < 1. The soft-x-ray emission (SXE) spectroscopy is a useful tool to investigate the chemical bonds of buried interfaces. Carlisle *et al.* [2] concluded from SXE spectra and near-edge absorption data that the spacer layer is metallic in antiferromagnetically coupled Fe/Si multilayers.

A series of Fe(30Å)/Si(t) multilayers were prepared using a dc magnetron sputter system under an Ar pressure of 1.6 mTorr. The temperature dependence of the resistivity perpendicular to plane measured for the multilayers showed that the Si layer was unambiguously an insulating layer. The antiferromagnetic coupling was observed for samples of 10Å < t < 15Å. Figure 1 shows the Si  $L_{2,3}$  SXE spectra measured for the multilayer samples and amorphous Si using electron beam excitation. They were fairly consistent with those obtained using SR. The spectral feature of the t = 40 Å sample is quite similar to that of amorphous Si. The peak at 90 eV and the shoulder at 98 eV become steeper with decreasing t, and the feature finally resembles that of Fe<sub>3</sub>Si. Thus the interface in the antiferromagnetically coupled sample (t=15Å) consists of metallic silicide, which cannot contribute to the interlayer coupling. Considering the resistivity property we speculate that the interlayer coupling originates from a very thin nonmagnetic and insulating layer sandwiched by the metallic silicide.

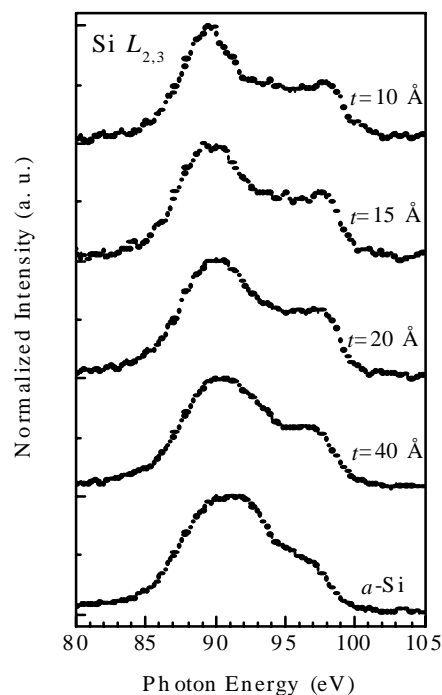


Figure 1: Si  $L_{2,3}$  SXE spectra measured for the Fe(30Å)/Si(t) multilayers and amorphous Si.

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- [2] J.A. Carlisle, A. Chaiken, *et al.*, Phys. Rev. **B53**, R8824 (1996).

# Defect-induced lateral heterogeneity at metal/n-GaN interfaces and its effect on the Schottky barrier heights

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Employing synchrotron radiation photoelectron spectroscopy, which provides chemical and electronic information from sub- $\mu\text{m}$  surface areas, has enabled us to identify composition heterogeneity developed at the metal/n-GaN interfaces and investigate its effect on the local Schottky barrier heights and surface conductivity. In all three cases, Au/GaN, Ti/GaN and Ni/GaN, the reaction-induced heterogeneity at the interfaces was related to the presence of defect areas in the GaN epilayers grown on different substrates. The most peculiar finding is that this inhomogeneity does not lead to the expected variations in the Schottky barrier heights. Detailed characterization of the interfaces was made in order to understand the effect of the interface morphology on the electronic properties of these interfaces.

Figure 1 shows an example the Ga 3d and Ni 3p maps from a ‘defect’ GaN region taken after Ni deposition and following annealing to 300 C for 120 sec. Spectroscopic examination was necessary to specify the origin of the observed contrast. The most peculiar finding is the presence of C in some microspots within the dark areas and the higher reactivity exhibited by the defect regions.

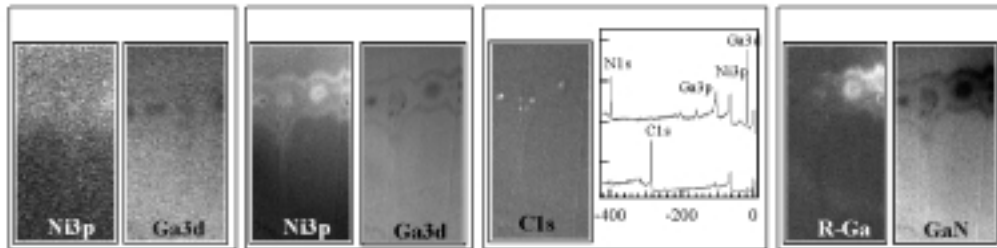


FIG. 1 Ni 3p and Ga 3d maps taken at 25 C (a) and after annealing to 300 C (b). (c) C 1s map and entire spectrum measured in the C spots (bottom) and in the non-defect region (top). (d) Ga 3d chemical maps illustrating the higher reactivity of the defect areas, right – image of reacted component, left – image of component from GaN.



## Surface Core Level Shifts of Clean and Oxygen Covered Ru(0001)

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Surface core level shifts (SCLS) measured at high resolution, as is now available at third generation synchrotron sources, can contribute valuable information on the charge rearrangements induced by the surface situation for clean surfaces, and by the presence of adsorbates. Even if measured with high resolution, the disentanglement of the observed shifts into contributions of initial state (charge redistribution in the ground state, including bonding) and of final state (charge redistribution in the core-ionized state, in particular screening changes) effects is difficult. Such an interpretation is possible if equally accurate and reliable calculations are available.

We have performed High Resolution XPS experiments of the Ru(0001) surface, either clean or covered with well-defined amounts of oxygen. For the clean surface we detected two distinct components in the Ru3d<sub>5/2</sub> core level spectra, for which a definite assignment was made using the High Resolution Angle-Scan Photoelectron Diffraction approach. The first principles all electron density functional slab calculations (LAPW code WIEN97, PBE-GGA) are in very good agreement with our experimental results. For the (2x2), (2x1), (2x2)3O and (1x1) oxygen structures we found Ru 3d<sub>5/2</sub> core level peaks which are shifted up to 1 eV. Again, very good agreement with the corresponding calculations results. Since the latter permit the separation of initial and final state effects, our coupled results give valuable informations for the understanding of bonding and screening at the surface otherwise not accessible in the measurement of the core level energies of the adsorbate.

# CHEMISORPTION AND SURFACE REACTIONS OF NH<sub>3</sub> ON Si(001)2×1 STUDIED BY HIGH RESOLUTION PHOTOEMISSION SPECTROSCOPY

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Reactions of ammonia on the Si(001) surface have a considerable importance since NH<sub>3</sub> is an excellent nitration agent and is the most frequently used nitrogen source for silicon nitride and silicon oxynitride CVD growth. In spite of the numerous investigations performed on the NH<sub>3</sub>/Si(001) system, a clear understanding of the bonding configurations assumed by N atoms on the silicon surface, especially in the intermediate stages between the initial chemisorption and the high temperature silicon nitride growth, has not yet been achieved. Concerning photoemission, differently from the NH<sub>3</sub> adsorption on the Si(111) surface, which has been recently studied with high energy resolution<sup>1</sup>, only studies performed at moderate energy resolution have been reported up to now in the case of the NH<sub>3</sub>/Si(001) interface and a unequivocal correspondence between the N bonding environment and the N 1s and Si2p core level shifts has not been obtained.

In this study the low temperature (150 K) adsorption of ammonia on Si(001)2×1 and the thermal reactions occurring up to 850 °C were studied by high resolution core level and valence band photoemission spectroscopy at the SuperESCA beamline of ELETTRA. Si2p and N1s core level components were correlated to the dissociative chemisorption and molecular physisorption occurring at low temperature, whereas at higher temperature monitored the transition from the initial NH<sub>2</sub> adspecies to N triply coordinated to Si. Results were compared with spectra taken on silicon nitride grown by dosing NH<sub>3</sub> on the surface held at 850 °C.

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# LAYER DEPENDENT PHOTOEMISSION IN ULTRATHIN Ar LAYERS ON Pt(111)

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Solid films of rare gases on metals are known to show layer dependent photoemission spectra. Recently in the case of Xe adsorbed on Pt(100)<sup>1</sup>, Ag(111)<sup>2</sup>, Cu(100)<sup>2,3</sup> and Ru(0001)<sup>3</sup> the thickness dependent changes have been interpreted as a quantization of the electron states perpendicular to the surface depending on the number of adsorbed layers.

Argon physisorbs on the Pt(111) surface forming ordered structures several monolayers thick. In this study we dosed with Ar the Pt(111) surface at 40 K and measured the evolution of the Ar2p, Ar3s and Ar3p spectra during gas adsorption using fast photoemission at the Superesca beamline of Elettra. The Ar 3p spectra measured at increasing Ar coverage and the Ar 3s isointensity plot up to an Ar dose of 4 Langmuirs are shown in Fig.1. Peaks corresponding to different layers are shifted in binding energy and decrease in intensity after the adsorption of an additional layer on top of the structure. Analysis of the layer resolved shifts within a potential well model for the quantization of the electron states is in progress.

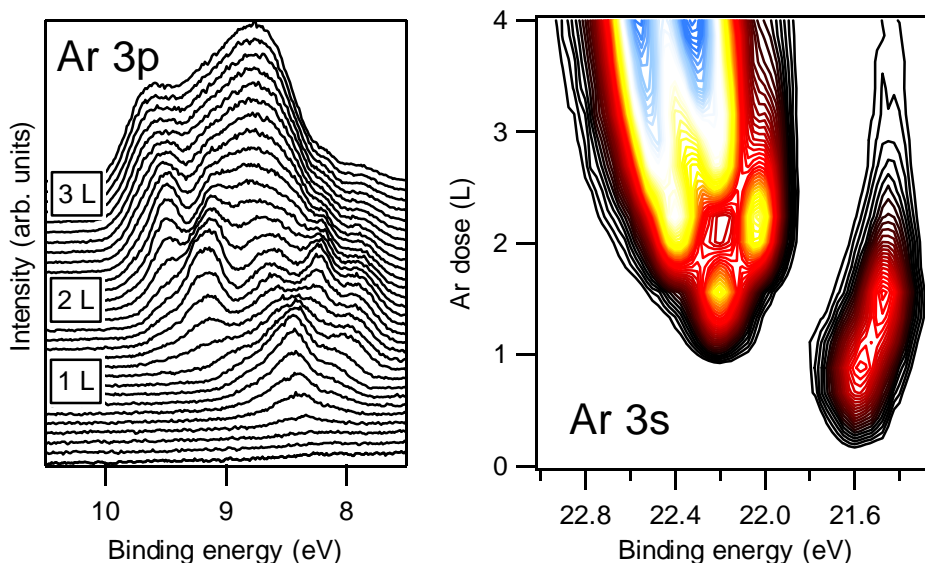


Fig.1 (left) Ar 3p spectra and (right) isointensity contour plot of the Ar 3s spectra taken during Ar adsorption on Pt(111) at 40 K using photon energy at 96 eV.

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# Spin reorientation transition induced by adsorption of H<sub>2</sub> and CO on Ni/Cu(001) observed by x-ray magnetic circular dichroism

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It is well known that magnetic metal thin films show unique properties such as perpendicular magnetic anisotropy (PMA). PMA has widely been investigated for technological and scientific researches. Recently, it was found that absorption of H<sub>2</sub> and CO on Ni thin films grown on Cu(001) causes a change of magnetization easy axis from in-plane to perpendicular [1]. In this work, we have measured Ni *L*-edge x-ray magnetic circular dichroism (XMCD) of Ni/Cu(100) before and after the spin reorientation transition induced by H<sub>2</sub> or CO adsorption.

All the spectra were taken at bending-magnet Beamline 7A of the Photon Factory. Ni films were grown by evaporation from resistively heating of wires, and thickness was controlled by in-situ monitoring reflection high-energy electron diffraction oscillation. We have prepared several films of 6-12 ML around which the transition from in-plane to perpendicular magnetization occurs. Subsequently, the film was dosed with H<sub>2</sub> at 200 K and with CO was 300K. The samples were magnetized by pulsed magnetic field and the remanent magnetization was investigated.

The Ni *L*-edge XMCD spectra were analyzed by using the sum rule for obtaining the spin and orbital magnetic moments ( $M_s$  and  $M_l$ ) separately. We have observed the spin reorientation transition from in-plane to perpendicular in the range of 7-9 ML after H<sub>2</sub> and CO adsorption. The critical thickness of clean Ni/Cu(100) is about 9 ML and that of H<sub>2</sub> or CO covered ones is about 7 ML. This means that H<sub>2</sub> or CO adsorption stabilizes PMA.

The ratio of the orbital-to-spin magnetic moment,  $M_l/M_s$ , before and after adsorption of H<sub>2</sub> is shown in Fig. 1. For the clean Ni films, the orbital magnetic moment is gradually enhanced as the film thickness decreases. Or rather, in the in-plane magnetized films with thickness less than 9 ML, the  $M_l/M_s$  ratio is enhanced compared to the PMA ones beyond 9 ML. After H<sub>2</sub> adsorption, all the films investigated here show PMA, and the  $M_l/M_s$  values are almost constant as a function of Ni thickness, as shown in Fig. 1. It is concluded that H<sub>2</sub> adsorption suppresses the orbital magnetic moment of Ni, this leading to the spin orientation transition from in-plane to perpendicular. The results of CO adsorption will also be presented at the Conference.

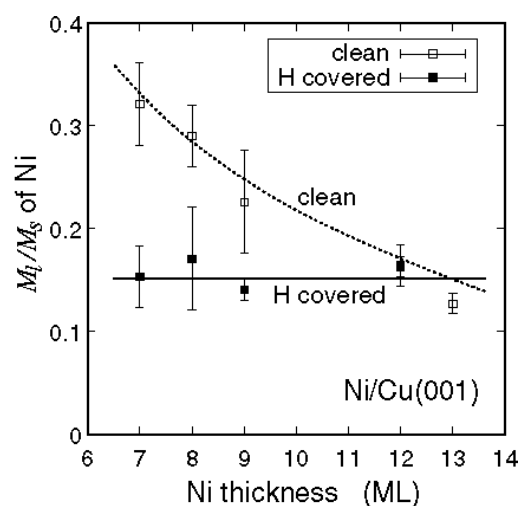


Fig. 1 The ratio of orbital and spin magnetic moments of the Ni thin films before and after H<sub>2</sub> adsorption..

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# The Effect of Multiple Scattering on the Circular Dichroism in Angular Resolved Photoemission from Molecular Adsorbates

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We report on the dichroism in angular resolved photoemission excited by circularly polarized light. The difference in the differential cross section determined for opposite helicity of the photons is usually termed CDAD (circular dichroism in the angular distribution). The CDAD was observed for emission from the N 1s core-level of NO molecules being adsorbed in a p(2x2) superstructure on Pt(111). The CDAD was measured in a plane perpendicular to the plane of photon incidence. It vanishes in normal emission, independent of the photon incidence. The azimuth of the sample was rotated so that different mirror planes coincide with the plane of observation. Differences in the CDAD are observed mainly at large polar angles.

The CDAD from K shells is expected to vanish identically if atomic models are recalled. Therefore, the CDAD was theoretically investigated using a three step cluster photoemission model. It was previously shown that the main aspects of the CDAD are already described by a single scattering formalism [1]. This single scattering model is extended to include multiple scattering. For the free NO molecule we present a model that includes an infinite number of scattering events. This model is used to explain how the CDAD changes if the number of scattering events is successively raised. Further it is used to explain basic effects of the molecular orientation. The Pt(111)-p(2x2)NO structure is modeled by a cluster of variable size to study the effect of multiple scattering on the CDAD from the complete adsorbate system. It is shown that the multiple scattering does not introduce new features in the angular dependence of the CDAD, it merely changes the absolute values. We conclude that the CDAD is much less sensitive to multiple scattering than the differential cross-section itself.

The calculations are compared to the measurements in order to determine the adsorption site and geometry. It is shown that already the single scattering approach confirms the on-top adsorption site with the N-end of the molecule bound to the Pt substrate. We will show how the CDAD measurements may be extended to allow a direct determination of the height of the molecule above the substrate. Finally a comparison to the CDAD measured from the C-1s and O-1s shells of CO adsorbed on Pd(111) will be given [2].

(This work is funded by the German government via BMBF - 05 SC8UMA0)

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# TEMPERATURE AND DEFECT DENSITY DEPENDENCE OF THE 1/3 ML Sn/Si(111) SURFACE

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The  $\alpha$  phase (1/3 of a monolayer (ML)) of Sn on Si(111) has been investigated as a function of temperature (40-300 K) and as a function of surface defect density (1-54 % of substitutional Si ad-atoms) by means of high resolution (40 meV) synchrotron radiation core level photoemission.

Although the LEED pattern shows a  $(\sqrt{3}\times\sqrt{3})R30^\circ$  periodicity and no sign of  $(3\times 3)$  reconstruction has been reported, we observed that Sn 4d core level spectra of the almost defect-free surface present two well-defined components shifted by 0.46 eV. The intensity ratio between these components is close to the expected ratio for a  $(3\times 3)$  periodicity (i.e. 2). These findings are substantially temperature independent (40-300 K) and suggest the presence of two non-equivalent  $T_4$  adsorption sites.

Increasing the surface defect density by annealing at different temperatures [1], the evolution of the Sn 4d line shape again indicates that only two components are present. There is no energy shift between these two components and the corresponding ones in the almost defect-free surface. The only main effect we observed is the progressive intensity reduction of the major component. In contrast with the suggestion of Uhrberg *et al.* [2], no spectral feature can be clearly associated to the Sn atoms around the Si defects. The onset of a  $(3\times 3)$  background in the 100 K LEED pattern has been observed only for a Si ad-atom concentration close to 25 %.

The XPS data will be also compared with corresponding STM images and an overall interpretation scheme will be given.

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# PHOTOEMISSION STUDY ON THE SURFACE RECONSTRUCTIONS OF Pb ON Si(100)

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Surface reconstructions induced by Pb adsorption on a Si(100) surface have been studied by high-resolution photoelectron spectroscopy using synchrotron radiation at a newly-built VUV beam line BL-1C at Photon Factory. The single-atom-wide chains of Pb adsorbates were identified in the Pb coverage range less than 0.5 monolayers (ML) at room temperature [1]. The Pb chains are proposed to consist of parallel buckled dimers by the scanning tunneling microscope study [1] and *ab initio* total-energy calculations [2] in contrast to the group-III adsorbate systems. There are also complex phases, c(4x8) and 2x1, beyond 0.5 ML. However, no detailed structural analyses were carried out to confirm these structures.

Figure 1 shows the Pb 5*d* spectra for the 2x2 and 2x1 phases taken at  $h\nu = 50$  eV with the results of corresponding curve fitting. The Pb 5*d* spectrum for the 2x2-Pb surface is decomposed into two components, indicating that the Pb chains consist of buckled dimers. On the other hand, The Pb 5*d* spectrum for the 2x1-Pb surface is found to consist of one dominant component, suggesting that the buckled dimers are not the major adsorbate configuration in the 2x1 unit cell. Moreover, the Pb 5*d* spectrum for the 2x1-Pb exhibits a long tail on the low kinetic energy side. This existence of the high asymmetric tail indicates a metallic nature of the surface, which is consistent with the previous study by angle-resolved photoelectron spectroscopy [3]. The Pb 5*d* and Si 2*p* core-level analyses of the Pb/Si(100) with different coverage are also discussed systematically.

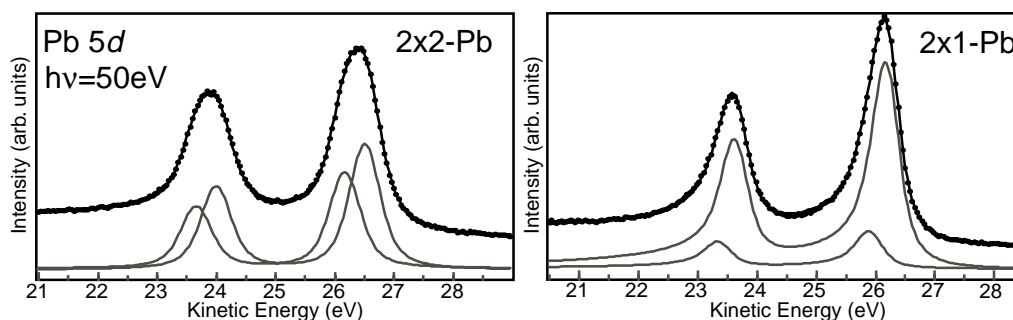


Figure 1: Pb 5*d* core-level spectra from both the 2x2-Pb and 2x1-Pb surfaces taken with photon energy ( $h\nu$ ) of 50 eV in normal emission ( $\theta_e=0^\circ$ ) with the results of curve-fitting analyses.

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# Overlayer Metallization of Na/Si(100) Surface

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Alkali metal (AM)/Si surface has received much attention as a model system of metal-semiconductor interface [1]. AM is known to reduce the work-function and act as a catalyst for the oxidation of silicon. There have been a number of studies concerning the bonding between AM and Si, AM coverage, and the surface metallization, etc. It has been widely believed that the adsorption of K (or Cs) on Si(100) surface gives rise to an overlayer metallization but the Na/Si(100) surface is semiconducting at room temperature [2]. To the contrary, some experimental results suggest that Na overlayer is also metallic. In this work, we provide an evidence for the overlayer metallization of Na/Si(100) surface.

The experiment was performed in an ultra-high vacuum chamber equipped with low energy electron diffraction and synchrotron radiation photoemission spectroscopy at the beam line 2B1 of PAL in Korea. We measured the change of work-function and core level (Si 2p, Na 2p) spectra with increasing Na deposition time. The work-function change decreased (to about 3.2 eV) linearly up to the saturation coverage. It should be noted that a structure appears and then grows up as the coverage increases. Its kinetic energy is independent of the incident photon energy and the structure is also found in Na thin films. These results suggest that the structure is a LVV Auger peak from metallic Na overlayer.

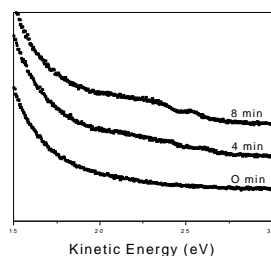


Figure 1: LVV Auger spectra taken from Na/Si(100) surface at several Na deposition time.

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# Electronic Structure of Ag Thin Films on Ge(001) Surface

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Ag deposited Ge(001) surface is known to show superconducting (SC) behaviors below ~8K. It is localized at surface since Ag and Ge are not superconductors. Recent scanning tunneling spectroscopy work showed non-linear I-V character, which supports SC, but the surface structure contributing to SC is still unclear [1]. So far, we have studied the initial growth of Ag by using scanning tunneling microscopy (STM) at room temperature (RT) and found two characteristic surface structures [2]. On the substrate at 90K, two dimensional (2D) monoatomic height Ag islands grow along the dimer-row. It is possible to saturate the substrate only with 2D islands at Ag thickness of ~2Å. Another is three dimensional (3D) islands which grow at RT. In the present work, we have studied valence band spectra and surface core-level shift (SCLS) to reveal the electronic structure of these two kinds of islands.

The experiments were performed at beamline 18A at KEK-PF. A clean Ge(001)-(2×1) surface was obtained by the repetition of Ar<sup>+</sup> ion sputtering and annealing at ~970K. Ag was deposited at substrate temperature of 90K and RT. The average thickness of Ag was 1 – 2.1Å. SCLS and valence band spectra were measured at RT for each sample. Figure 1 shows Ge 3d spectra. A shoulder at lower binding energy on clean surface (A in Fig.1 (a)) is suppressed in the case of low-temperature Ag deposition (Fig.1 (b)). This suggests a strong interaction between Ag and the substrate. In the valence band spectrum (Fig.2 (b)), all the surface states on the clean surface (S<sub>1</sub>–S<sub>4</sub> in Fig.2 (a)) are suppressed and some new features (indicated by arrows) appear. Increment of the density of states just below Fermi level and atomic Ag 4d peak are also found. In the case of RT deposition (Fig.2 (c)), surface states on the clean surface still remain. Ag 4d has wide bandwidth and show bulk-like character. The shoulder in Ge 3d spectrum also remains (Fig.1 (c)) and suggests the growth of 3D islands which have not saturate the substrate. These findings are consistent with the STM observation.

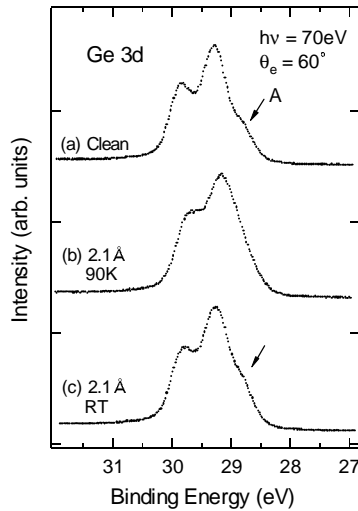


Figure 1: Ge 3d spectra for (a) clean surface, (b) 2.1Å deposited at 90K, (c) 2.1Å deposited at RT.

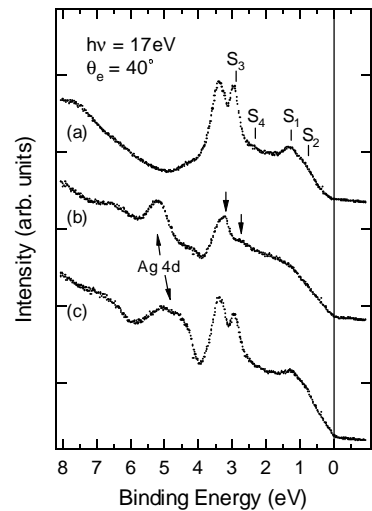


Figure 2: ARPES spectra for (a) clean surface, (b) 2.1Å deposited at 90K, (c) 2.1Å deposited at RT.

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# THEORY AND X-RAY ABSORPTION SPECTROSCOPY OF THE SIGMA-SHAPE RESONANCE OF LINEAR HYDROCARBONS.

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One of the very useful successes of the X-ray absorption spectroscopy is the study of molecular excitations close to the absorption edge. This may be the transition of  $1s^{-1}$  to unoccupied bound states (e.g. LUMO) or to quasibound states in the continuum. Full use of the linear polarized synchrotron radiation can be made if the molecules are aligned, i.e. oriented on a surface and not random as in the gas phase.

We present new results for NEXAFS (XANES) of the  $\sigma^*$  shape resonance for the linear hydrocarbon molecules ethane ( $C_2H_6$ ), ethylene ( $C_2H_4$ ) and acetylene ( $C_2H_2$ ), adsorbed on a Cu(100) surface. These molecules play an important part in the discussion concerning the so-called  $\sigma^*$  shape resonance, as they can be considered a paradigm for systems with a single, double and triple bond, resulting in a systematic variation of the C-C bond length  $d_{c-c}$ . This new analysis is combined with first principle calculations of the total absorption cross section. The theory is based on a relativistic Green's function formalism, using an *ab initio* self-consistent field (SCF) real space multiple scattering (RSMS) approach for a defined cluster of about 100 atoms. The SCF potentials are essential for an accurate determination of the Fermi level. For the purpose of an improved calculation of NEXAFS spectra, a full multiple scattering (FMS) approach is implemented into the code. FEFF8 calculates the excitation of a photoelectron of the cluster for a fully relaxed core hole.

For a critical comparison between theory and experiment it is important to calculate and measure the total cross section  $\mu(E, \Theta, T)$ , that is to say to follow the angular dependence for an E1 transition and to take into consideration the thermal damping of the resonance. Moreover it is insufficient to discuss only the energy position of the resonance, more important is to calculate and measure the asymmetric resonance profile, which is a principle feature when scattering into the continuum.

Both, theory and experiment, are in excellent agreement [1,2]. Other work addressing the same question will be discussed as well. The present work will serve to bring the X-ray absorption spectroscopy on a level of a more quantitative analysis and principle understanding, getting away from finger print assignments.

This work was supported by BMBF grant# 05 SF8 KEA 2

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# ELECTRONIC STRUCTURE OF THE Si(001)5x3.2-Au SURFACE

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Au adsorption on Si surfaces has been one of the prototype systems for understanding fundamental physical properties of metal/semiconductor interfaces. Although intensive studies have focussed on Au/Si(111) surfaces, recently there have been growing interests in Au/Si(001) surfaces. In the initial stage of Au adsorption on the Si(001) surface, several long-ranged ordered phases such as 5x3.2 are formed. However, up to now, there is no electronic structure study on Au/Si(001) surfaces. In this research, electronic structure of the Si(001)5x3.2-Au surface was investigated by angle-resolved photoelectron spectroscopy using synchrotron radiation. The experiment was performed on the beam line 7B at Photon Factory in Japan.

From detail measurements, the dispersions and symmetries of surface states were determined for the highly symmetric axes of surface Brillouin zones (SBZs). The surface state dispersions of Si(001)5x3.2-Au are shown in figure. The surface is metallic with a shallow metallic state ( $m_1$ ) dispersing anisotropically. The dispersion of  $m_1$  is, however, found not to coincide with the periodicity of the SBZ along  $[110]$  direction. In the figure, the presence and dispersions of three other surface state bands,  $S_1$ ,  $S_2$  and  $S'_2$ , are also identified within the band gap. These results are discussed by comparing with those of the recent structure studies of this surface.

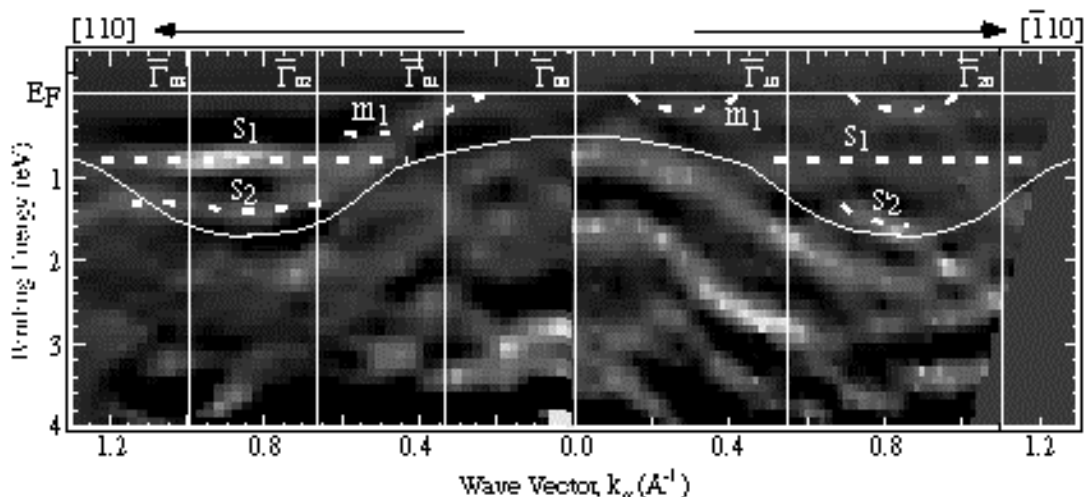


Figure: Gray-scale  $E_B$ (binding energy)- $k_{//}$ (wave vector) diagram for the Si(001)5x3.2-Au along  $[110]$  ( $h\nu = 21.9$  eV) and  $[\bar{1}10]$  ( $h\nu = 17.0$  eV) directions. The dispersions for the surface states are depicted as white dashed curves. The white solid curve is the edge of bulk band projection into  $1 \times 1$  SBZ.

# Interatomic Phenomena in Resonant Photoemission from Adsorbate Layers on Ni(111)

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In this contribution we address the effect of interatomic multi-atom resonant photoemission (MARPE) in adsorbate layers. MARPE has recently caused a lot of interest, first when it was observed [1], and second when problems with detector non-linearities questioned the effect as being induced by the experimental equipment [2,3]. In principle, MARPE should be observed when the photon energy is tuned to a core-level absorption edge of an atom A neighboring the atom B from which the photoelectron is detected [1].

We have studied this phenomenon for adsorbates on Ni(111) with varying bond strengths to the surface. Starting from CO, i.e., fairly strong chemisorption, we investigated physisorbed systems like Ar, N<sub>2</sub>, N<sub>2</sub> on Ar, and CO multilayers. Using the detector at the SUPERESCA beamline at ELETTRA (Trieste) with its confirmed strict linearity in counting efficiency, allows us to unambiguously measure even small effects. For all systems studied we obtain a very similar behavior. Measurements performed at normal incidence of the synchrotron light show a reduction of the respective core level intensities (C 1s, O 1s in CO, Ar 2p, N 1s) by about 10% when tuning the photon energy across the Ni L3 edge at about 855 eV. Going to grazing light incidence (10°) we find a decrease of the signals by about 25%, again independent of the system. In terms of resonant photoemission, the profile can be described by a q-value close to q=0, as expected for direct photoemission being the dominant channel.

Since even the decoupled system of N<sub>2</sub> on Ar on Ni(111) showed the same magnitude of the effect as the truly chemisorbed CO/Ni(111), the observed intensity variation cannot depend on the overlap of wave functions. Also, the distance between the two atoms involved does not play a significant role either. The trend in the observed variation of the effect with light incidence angle would support the explanation of MARPE in terms of x-ray optics, taking the change in the absorption coefficients at strong absorption edges into account [2]. That way, the results would also be independent of adsorbate and only depend on the substrate used. However, from a previous account of this theoretical description [2] one would conclude, that at normal incidence the observed effect should be much smaller than observed here, which calls for further theoretical work.

This work was supported by EU ARI program (HPRI-CT-1999-00033).

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## Quantum Size Effect on Pb/Ge(100) system

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When electronic states are confined in the z-direction of a thin film they become discretized, a continuous band splits up into discrete points in the slab and their number increases by increasing the film thickness [1,2]; the quantization is due to the confinement of the wavefunction inside the slab. The quality of the interface between the metal film and the substrate material plays a crucial role in the observation of the effect.

From the structural point of view we found that the deposition of lead on the c(4x2)Ge(100) double domain surface, for film thickness above 3 ML at 100 K, leads to a layer by layer Pb film growth, with a double domain (111) structure as shown by LEED, in agreement with Helium Atom Scattering (HAS) experiments [3]. Early stages of Pb growth lead to an intermediate phase that should correspond to intermixing of Pb and Ge. This phase shows a complex LEED, different by the pseudomorphic (4x1) superstructure already detected in the literature [4] and is probably the evolution from the (100) to the hexagonal symmetry.

We performed angle-resolved photoemission measurements, at the VUV beam line of ELETTRA, to study the quantum size effect on thin films of Pb deposited on Ge(100) c(4x2) surface at low temperatures (100K). Quantum Size States (QWS) are unambiguously pointed out as a series of peaks in Valence Band (VB) below EF for film thickness ranging between 3 and 20 ML. We measured the VB spectra as a function of the film thickness, and of the emission angle (in ARUPS spectra) in order to detect the dispersion of the QWS. The number of the QWS increases with the number of layers and their energy position moves towards the upper band edge as a function of the film thickness "d". As a consequence the intensity at Fermi level changes periodically as a function of "d", reaching a maximum at some particular values.

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# Changes induced in the surface electronic structure of Be(0001) after Si adsorption.

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Effects induced on the surface electronic properties of Be(0001) upon Si adsorption have been investigated. One motivation was that epitaxial Be(0001) films grown on Si(111) substrates showed significantly different electronic properties [1] compared to the (0001) surface of bulk single crystals [2,3]. Segregation of Si to the surface was suspected to be the reason for these differences. Therefore a core level and valence band study of Be(0001) single crystal surface after deposition of Si overlayers at room temperature and after subsequent heating was made. After deposition a 1x1 LEED pattern with weak  $\sqrt{3}\times\sqrt{3}$  R30° spots [4] was observed. After heating to about 450 C° the  $\sqrt{3}$  spots were no longer visible.

The four surface shifted Be 1s levels on the clean Be(0001) surface [2] showed after deposition pronounced differences in relative strengths and after heating both the number of resolved surface components and the shifts were found to be smaller. Thus a small amount of Si in the surface region was found to have a dramatic effect on the surface shifted Be 1s core levels. The Si 2p level was after deposition quite broad and showed presence of more than one component. After heating the Si 2p spectrum contained essentially only one component.

The prominent surface state [3] at the  $\Gamma$  point on the clean Be(0001) surface was found to broaden and weaken considerably after Si deposition. After heating it was found to shift downward in energy by about 1.2 eV. The dispersion of this surface state was mapped over the Surface Brillouin Zone and showed fairly great similarities with the dispersion reported for Be(0001) with H [5] or Li [6] adsorbed on top.

These results will be presented and discussed.

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# SPIN-RESOLVED PHOTOELECTRON SPECTROSCOPY OF ULTRATHIN FE FILMS ON GAAS(001)

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Thin epitaxial Fe films were grown on singular and vicinal GaAs(001) substrates, and their magnetic and electronic structure were investigated by a synchrotron based spin-resolved and spin-integrated photoelectron spectroscopy with different Fe thickness[1]. There were two types of substrates; one was a Si-doped n-type GaAs(001) surfaces with doping concentration of  $2 \times 10^{18} \text{ cm}^{-3}$  (hereafter, singular substrate), and the other was orientated by  $3^\circ$  towards (111)A direction (hereafter, vicinal substrate). Figure 1 shows typical spin polarization of the secondary electron peak with the growth of Fe coverage for the singular substrate sample and the vicinal one. In the case of singular substrates, there was a dependence of their initial surface reconstruction, which is associated with complex domain structure [2], while no such the dependence was observed in the case of vicinal substrates. The result from the vicinal sample suggests that the geometrical influence of the initial surface stoichiometry of the substrate. In this paper, further latest results of the rotation of the spin polarization and change of core level peaks are also reported.

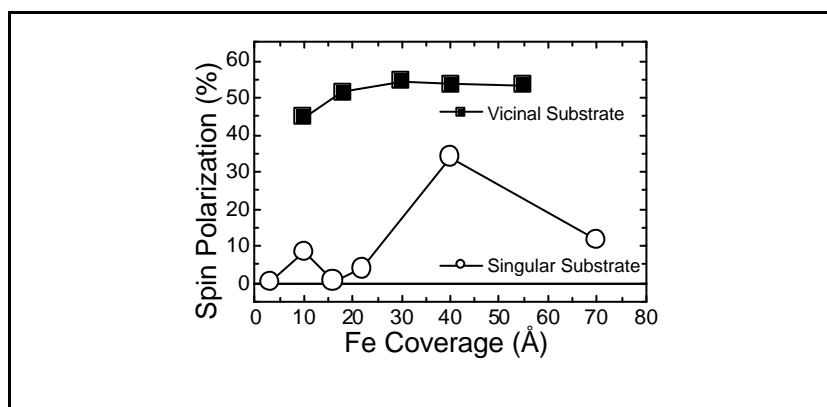


Figure 1: Spin polarization of secondary electrons as a function of Fe coverage. Black square for the vicinal substrate, and open circle for the singular substrate.

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# INTERFACIAL REACTION AT NI(FILM)/4H-SiC(SUBSTRATE) SYSTEM STUDIED USING SOFT X-RAY EMISSION SPECTROSCOPY

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Silicon carbide (SiC) is a suitable semiconductor for electronic devices operating at high temperatures and at high power. Knowledge of how metal/SiC interfaces are affected by elevated temperatures is required since the performance of the devices strongly depends on the electronic properties of metal/semiconductor contacts. Also metal silicides are of interest for contact materials for SiC device fabrication. Currently much of the mechanism of contact formation, especially the thermally induced chemical behavior at the interface region, is not adequately understood.

Soft x-ray emission spectroscopy (SXES) is a non-destructive, less surface sensitive method that provides information on valence features of the materials under investigation. Thus we can obtain the chemical information from buried interface region. Synchrotron radiation as an excitation source for SXES takes advantages such as high intensity, element selective excitation, and more non-destructive character compared with excitation by high-energy electron irradiation. The objective of this study is to analyze the interfacial reaction of thermally treated metal(Ni)/semiconductor(SiC) system qualitatively, using synchrotron radiation excited SXES.

Samples were prepared as follows: a Ni films with thickness of 30nm was deposited on a clean surface of n-type 4H-SiC (Cree Research Inc.) and annealed in N<sub>2</sub> + H<sub>2</sub> for 30min. The samples were characterized using SXES. SXES measurements were carried out at BL19B at Photon Factory, KEK, Japan.

Certain interfacial reaction was found to be induced by thermal annealing, and Ni Silicide formation was identified by the Si  $L_{2,3}$  emission band spectra. The existence of carbon species in the reacted region was indicated by the C  $K$  emission band spectra, and the chemical bondings of these C atoms differ from that of C in bulk SiC.



# Temperature and time dependence of emission properties of ZnO Films

## Deposited on Si Substrates

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Zinc oxide is a versatile material that has been applied as piezoelectric materials, gas sensors, buffer layer of GaN and surface acoustic wave devices. Recently, great interest has been paid to the emission properties of ZnO film, especially optically pumped UV lasing at RT,<sup>1</sup> because development of short-wavelength optical devices is highly desired for future opto-electronic technical industries.<sup>2</sup> In this paper, the emission properties of ZnO films deposited on Si substrates by reactive dc sputtering<sup>3</sup> has been studied using synchrotron radiation (SR) light source at HASYLAB, Germany. The integrated luminescence spectra as well as the spectra at a fast time window from about 4ns to 4ns and a slow time window from about 20ns to 140ns were measured simultaneously, at temperature range from several K to 350K. Apart from the free-exciton recombination (peaked at 369.5nm) and ultraviolet emission band (peaked at 390 nm) and green band (peaked at 520 nm), a new emission band peaked at 290 nm was found for the first time under SR vacuum ultraviolet excitation. The 290nm emission existed at temperatures below 180K only, while the 520nm emission appeared at temperatures higher than 180K. From the variation of the luminescence spectra in different time windows, it can estimated that the lifetime of the free-excitons is about several nano-seconds, the lifetime of 290nm emission is about several ten nanoseconds, and the lifetime of 380nm emission is much longer than 200 nano-seconds.

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## XPS and XAES study of carbon states on the surface of Pt(111)

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During the last decade chemistry of carbon had a good progress. The understanding of nature of carbon depositions on the platinum surfaces is very important for catalysis of hydrocarbon refining. The adsorbed layers of carbon on the surface of Pt(111) have been studied with aid of the photoemission methods (XPS and XAES). Carbon deposition was performed *in situ* in electron spectrometer VG ESCALAB by decomposition of simple hydrocarbons: methane or ethylene. Since dehydrogenation of hydrocarbons on Pt(111) occurs below 700 K, the catalytically obtained adsorbed layers studied in the temperature range 900–1400 K do not contain hydrogen or hydrocarbon species.

Photoemission spectra of carbon adsorbed layer obtained at  $T < 1100$  K characterize graphite-like structures. At temperatures being higher than 1100 K the structure of carbon adsorbed layer depends on carbonizing agent. In Figure 1 C1s and C-KLL spectra of two adsorbed layers obtained with usage of methane or ethylene at  $T = 1370$  K are presented. When methane is used for carbon deposition the electron emission characteristics ( $E_b(\text{C1s})$ , shake-up satellite structure, C-KLL shape) are practically the same as for graphite (curves 1). Otherwise, when ethylene is used, the spectroscopic characteristics are noticeably different (curves 2). The precise comparison with electron spectra obtained for carbon materials of different structure (HOPG, diamond, nanotubes, fullerenes) shows strong coincidence with spectra for fullerenes [1]. So, the formation of fullerite type adsorbed layer of carbon deposited from ethylene is proposed.

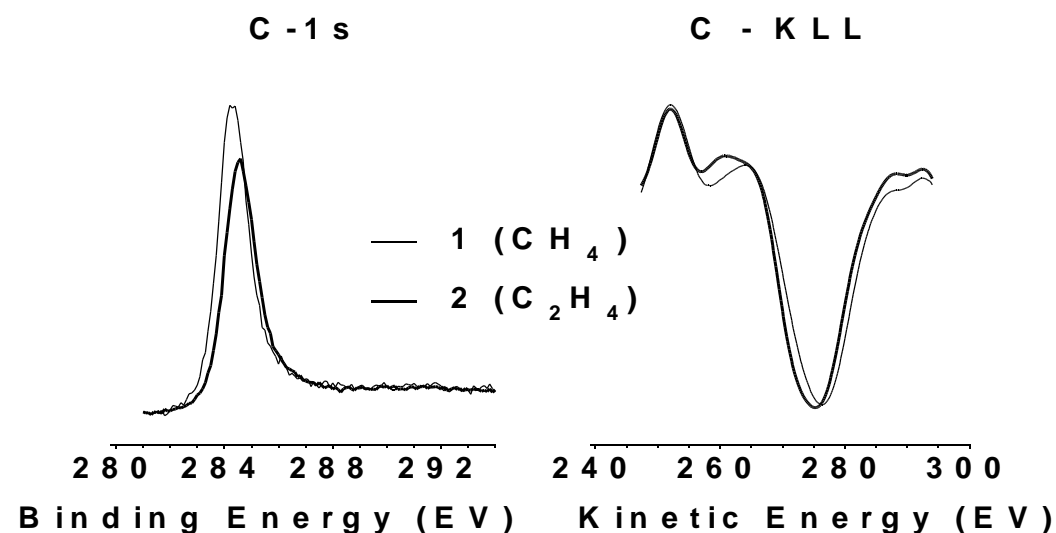


Figure 1. C1s and C-KLL spectra obtained for adsorbed layers of carbon deposited from methane and ethylene.

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# Dynamics of a thin Pd overlayer on a polycrystalline Ni surface

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In recent years, there has been considerable interest in the study of thin metal films deposited on metallic surfaces [1]. Polycrystalline substrates are interesting because they are closer to the materials used by industry than oriented monocrystals; indeed features such as grain boundaries strongly influence the behaviour of thin overlayers [2]. Photoemission microscopy with sub-micron spatial resolution is one of the most powerful techniques suitable for the study of these processes. The Scanning Photoemission Microscope (SPEM) installed at the ESCAmicroscopy beamline on the Elettra synchrotron light facility allows the acquisition of chemical maps using the core levels of a great number of metals, with a spatial resolution of 90 nm. The same instrument can also record photoemission spectra (with ~350 meV energy resolution) of the core levels and the valence bands from small areas of interest identified by means of the images.

In this work we present the results obtained after depositing and annealing a thin film of Pd (1ML) on a polycrystalline Ni sample. To simplify the data analysis we also identified the plane orientation of the crystals measured using the microLEED option of the SPE-LEEM microscope under commissioning at the NANOSpectroscopy beamline at Elettra. The images and spectra collected show a heterogeneous chemical behaviour of the Pd film on the different crystals, as can be seen from the figure 1. Closer inspection of the grain boundaries suggests that the Pd tends to migrate away from them.

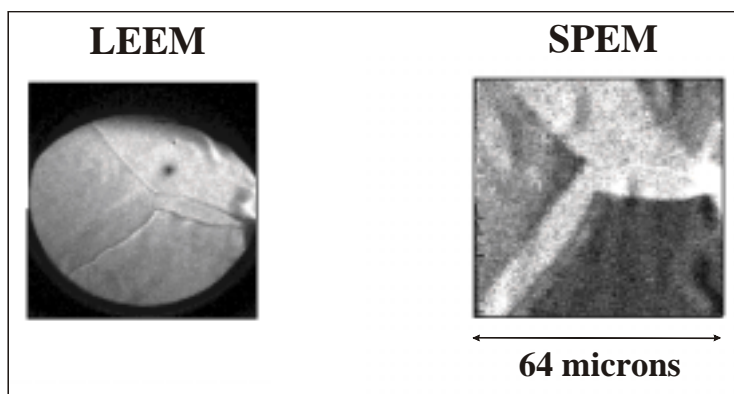


Figure 1: the left picture shows a LEEM image of a small portion of the Ni polycrystalline sample; a few grain boundaries that delimit different grains are clearly visible. The right image is a photoemission picture of the same area acquired using the Pd 3d core level signal. This image was taken after room temperature deposition of a thin (1 ML) Pd overlayer, and subsequent annealing at 720 K for 40 minutes.

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## Electronic properties of CaF<sub>2</sub> on Si(001)

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Due to the small lattice mismatch between the two materials (6% at room temperature), CaF<sub>2</sub> films of good crystal quality can be grown by MBE epitaxy on Si surfaces. CaF<sub>2</sub> is an insulator with a good optical transmission in the range of infrared and visible radiation. Epitaxial films of CaF<sub>2</sub> on Si, grown at elevated temperatures in UHV conditions, can be considered as promising candidates for substituting SiO<sub>2</sub> in MOS technology and in the fabrication of epitaxial multilayer structures [1], with possible applications in MISFETs and CCDs. Furthermore, films of CaF<sub>2</sub> on Si, if properly doped with rare earths and annealed at suitable high temperature, permit to realize solid state light emitters in the infrared and visible light ranges [2]. Under suitable growth conditions, CaF<sub>2</sub> nanostructures of different shape and size can be obtained on Si(001). Recently, CaF<sub>2</sub> grown on a Si(001) vicinal surface in a wide temperature range has permitted to realize nanostructures of different shape and dimensions (nanodots and nanowires) [3]. On the other hand, the interaction between a polar insulator with ionic bonding and a semiconductor with covalent bonding rises interesting questions about the interface bonding.

Angle resolved photoemission is used to get insights into the orientation of the CaF<sub>2</sub> molecules at the interface, on the chemical bond between the molecule and the substrate, and on the dependence of the electronic properties on nanostructures size when CaF<sub>2</sub> is grown on Si(001).

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# CORE LEVEL SHIFTS OF ORGANIC MOLECULES ADSORBED ON Si(100)-(2x1): A COMPARISON.

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Although many aspects of the adsorption of small hydrocarbon molecules on Si(100) have been quite extensively investigated, there is a lack of detailed information on the core level binding energies which can supply information on adsorbate-induced charge redistribution in the ground state and screening changes. We have therefore investigated different adsorbate systems under otherwise identical conditions: Adsorbate C 1s and substrate Si 2p core level binding energies for adsorption layers of six unsaturated hydrocarbons (C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>4</sub>, C<sub>4</sub>H<sub>6</sub>, C<sub>6</sub>D<sub>6</sub> (C<sub>6</sub>H<sub>6</sub>), and 1,2-C<sub>2</sub>H<sub>2</sub>Cl<sub>2</sub>) on a vicinal single-domain Si(100)-(2x1) surface have been determined by high resolution X-ray photoemission spectroscopy using synchrotron radiation. Results for the clean and the (2x1)-H covered surface have been obtained for comparison. Remarkable differences in the Si 2p and C 1s surface core level shifts for the various adsorbates are found, which range from 327 to -169 meV and from 1220 to -260 meV, respectively [1]. Both initial and final state effects are necessary to explain the strong but unsystematic variations of the observed shifts. Additionally, from a comparison of the C 1s intensities the absolute saturation coverages are determined.

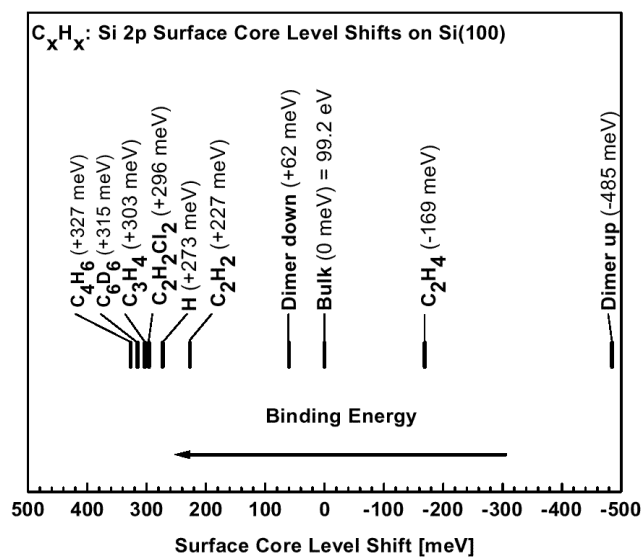


Figure 1: Surface core level shifts for different hydrocarbon adsorbates on Si(100)-(2x1). The Si 2p<sub>3/2</sub> core level bulk value is set to zero.

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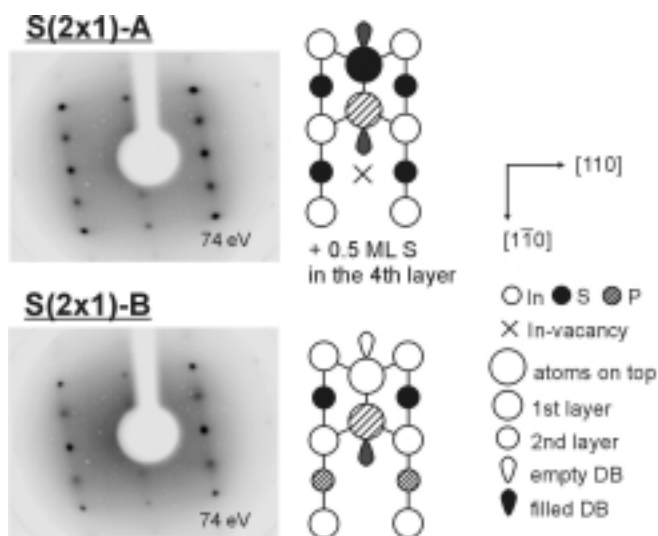
## TWO TYPES OF SULFUR-INDUCED (2×1) SUPERSTRUCTURES ON INP(001)

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Despite the ten-years story of intensive investigations, the atomic arrangement at the sulfurized InP(001)-(2×1)S surface is still far from clear understanding. In attempt to provide new information on this controversial issue we propose in this work a new method of surface sulfurization based on *in-situ* deposition of small amounts PbS onto the InP(001)-(2×4) surface followed by mild annealing to get rid of metallic lead and lead sulfide. It is shown that different steps of annealing of the surface prepared in this way



**Fig. 1** Two types of the sulfur-induced (2×1) superstructures on InP(001): LEED images and structural models.

can result in the formation of two different types of sulfur-induced (2×1) superstructures depending on the annealing temperature. The most probable structural models for both S(2×1)-A and S(2×1)-B superstructures are shown in Fig. 1. They are constructed on the basis of our XPS, LEED and ARUPS investigations. The S(2×1)-A reconstruction has been observed in the wide annealing temperature range of 200-400°C with the surface being free from any traces of Pb or PbS at 350-400°C. The proposed model of the corresponding surface structure implies formation of (2×1) surface unit cells with 1 ML of sulfur incorporated into the second layer on phosphorus sites and with a P-S dimer per cell along [1 $\bar{1}$ 0] (Fig. 1). The S(2×1)-B reconstruction appears in a narrow temperature range of 420-445°C and is assumed to possess the same atomic structure as the (2×1)-reconstruction typically observed on (NH<sub>4</sub>)<sub>2</sub>S-treated InP(001) above 360°C [1]. Further heating results in formation of regularly arranged surface domains of the S(2×1)-B phase and areas free of sulfur. Above 490-500°C no sulfur can be detected by XPS any more. Some number of In-vacancies in the third surface layer are probably necessary to conform the proposed models at least for S(2×1)-A to the electron counting rule. A detailed description of both sulfur-induced (2×1) superstructures observed upon PbS-sulfurization of InP(001) will be presented elsewhere [2].

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# SHIFT OF Fe $L_3M_{45}M_{45}$ AUGER SPECTRA WITH PHOTON ENERGY ACROSS Fe $L_2$ EDGE IN ULTRATHIN Fe FILMS ON CU(100)

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X-ray excited  $L_3$ - $M_{45}M_{45}$  Auger spectra of Ni, Cu and Zn show prominent satellites at low kinetic energies [1-3], which have been attributed to  $L_3M_{45}$ - $M_{45}M_{45}M_{45}$  Auger transitions in the presence of a 3d spectator hole. The  $L_3M_{45}$  doubly ionized initial states can be created by several mechanisms, in particular by  $L_1$ - $L_{23}M_{45}$  and  $L_2$ - $L_3M_{45}$  Coster-Kronig (CK) transitions and by  $L_3M_{45}$  shake up and shake off processes. Previous synchrotron radiation studies showed that in pure Fe the intensity of the  $L_3M_{45}$ - $M_{45}M_{45}M_{45}$  Auger vacancy satellite transition is negligibly small, because of a high degree of delocalization of the 3d spectator hole prior to the decay of the  $L_3$  core hole [4,5]. In FeAl alloys, instead, this transition has a significant intensity, since in this case the 3d spectator hole is more localized [5].

We investigated the presence of satellites in the  $L_3$ - $M_{45}M_{45}$  Auger spectra of ultrathin (1-2 ML) Fe films grown on Cu(100) by scanning the photon energy through the Fe  $L_2$  absorption edge and by Auger-photoelectron coincidence spectroscopy (APECS) experiments performed at ALOISA beamline, ELETTRA synchrotron radiation source. The aim of the experiments is to investigate a possible modification of the correlation effects consequent to reduced atomic coordination in the Fe films with respect to bulk Fe. The kinetic energy of the centroid of the Fe  $L_3$ - $M_{45}M_{45}$  feature has been found to disperse with photon energy, in a range covering Fe  $L_2$  absorption white line. The CK preceded contribution to the  $L_3$ - $M_{45}M_{45}$  Auger transition has been separated by detecting the  $L_3$ - $M_{45}M_{45}$  spectrum in coincidence with Fe  $2p_{1/2}$ . The feasibility of an APECS experiment on ultrathin films has been shown for the first time. We could observe the spectral lines resulting from coincidence between  $L_{23}$ - $M_{45}M_{45}$  and  $2p_{1/2}$  and  $2p_{3/2}$  photoionization events, respectively. The statistics of the data did not allow to observe a marked difference between the two cases, apart from the  $L_2$ - $M_{45}M_{45}$  contribution in coincidence with the ionization of the  $2p_{1/2}$  core level.

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# Structural transition in epitaxial Fe/Ni(111) films: from pseudomorphic fcc to NW-oriented bcc(110) phase

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Fe films epitaxially grown on fcc substrates represent a very attractive topic due to the strong interplay between structural and magnetic properties in Fe metastable fcc ( $\gamma$ ) phase at room temperature (RT) [1,2]. In this contribution we present a detailed structural study of Fe epitaxial films grown on Ni(111) at RT, performed by angle-scanned Photoelectron Diffraction (PD) with multiple scattering calculations' data modelling. Both back- and forward-scattering energy regimes have been employed in order to enhance structural sensitivity at lower and higher film thickness, respectively. We found that Fe atoms in the first layer occupy fcc hollow sites, and stack with pseudomorphic fcc structure up to 2 ML (see fig.1). Concerning the growth mode, evidence of good wetting and sharp Fe/Ni interface formation was observed. From 3 to 6 ML transition to bcc(110) phase develops. Quantitative R-factor analysis revealed that bcc(110) phase has Nishiyama-Wassermann (NW) in-plane orientation ( $\langle 001 \rangle_{\text{bcc}}$  directions parallel to  $\langle 1\bar{1}0 \rangle_{\text{fcc}}$  ones), with three non-equipopulated domains. The vertical interlayer distance between bcc(110) planes is  $d=2.11 \text{ \AA}$  (+3.9% expansion) at 6 ML and relaxes to  $d=2.05 \text{ \AA}$  (+1%) at 18 ML. In the same coverage range the angle between surface unit cell vectors changes from  $68^\circ$  to  $69^\circ$ , corresponding to -1.7 % and -1.0% contraction of cell area, respectively. Preliminary results from Surface X-Ray Diffraction data will be also presented to support the observed fcc(111)-bcc(110) NW structural transition.

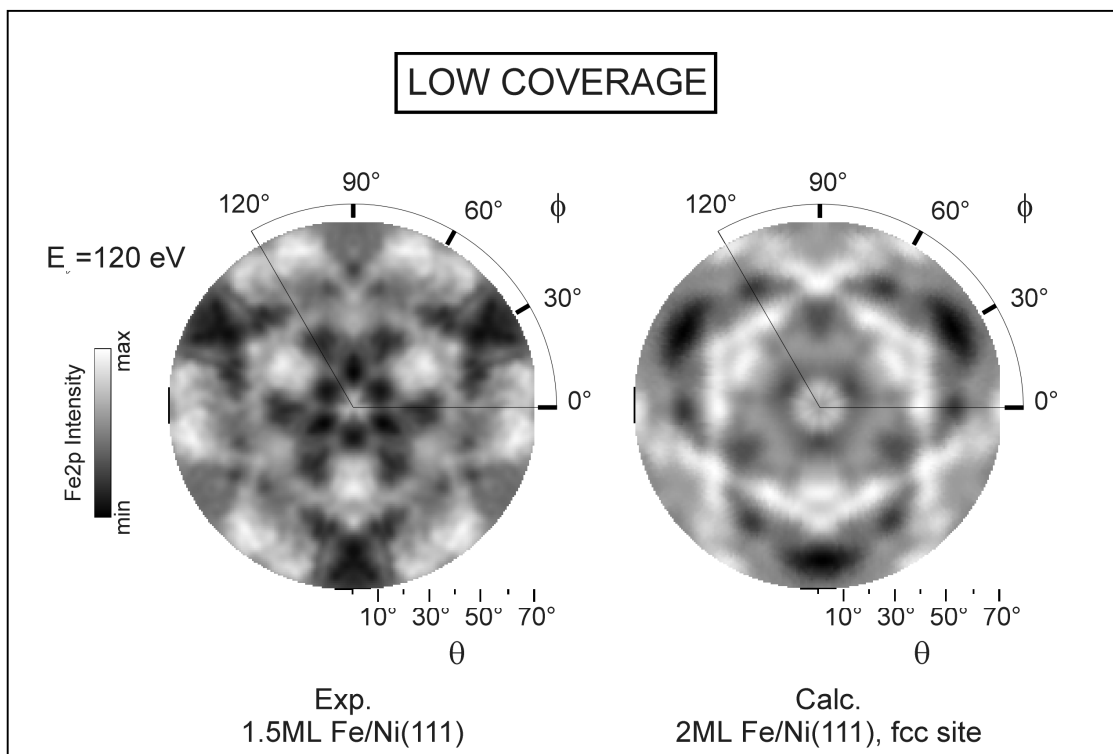


Fig. 1: **Left:** Stereographic projection of Fe2p intensity measured from 1.5 ML Fe/Ni(111) film in backscattering energy regime ( $E_k=120 \text{ eV}$ ). **Right:** multiple scattering calculation for a 2 ML film with Fe atoms at the interface occupying fcc hollow sites.

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## The Successive Metal - Insulator – Metal Transitions on the Si(111)7×7 Surface with K Overlayers

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A study of electronic band structure has been carried out for K adsorption on the metallic-like Si(111)7×7 surface in submonolayer coverage region. A new photoemission technique has been employed for probing surface band structure near both the Fermi level and valence band maximum (VBM) and for measuring the ionization energy and work function as a function of coverage. The technique of threshold photoemission spectroscopy is based on the separation of surface and bulk photoemission and on the near-threshold enhancement in photoemission from surface states by the quasi-resonant p-polarized light excitation [1-2].

Qualitative changes have been observed in the character of the electronic surface structure depending on K coverage. At low coverage  $\Theta < 0.15\text{ML}$ , one K-induced surface band below the VBM indicating the energy gap is revealed. Therefore, the suppression of metallic-like properties of the Si(111)7×7 surface due to K adsorption is observed in accordance with [3,4]. The metal-insulator transition is provided by disappearance of  $S_I$  surface state associated with Si “adatom” dangling bonds. No interaction between adsorbed atoms and Si “rest-atom” dangling bonds was found. Increasing K coverage leads to significant movement of the K-band towards the Fermi level. Before the saturation, the edge of K-band is found to be 0.45 eV above the VBM. The K/Si(111)7×7 interface is found to be semiconducting up to saturation coverage  $\Theta \sim 0.5\text{ ML}$ . Near saturation, K adsorption leads to drastic change in the surface band structure. The K-induced band crosses the Fermi level. Such surface band structure is identified as being metallic-like. The metallization is accompanied by the Fermi level pinning. Therefore, two surface transitions such as metal-to-insulator and insulator-to-metal are revealed.

A model taking into account local interactions between 6 K atoms and 12 Si “adatom” dangling bonds is developed for 2D system. The important role in such interaction can be caused metal cluster formation in the 7×7 unit cell through specific “Negative-U” effect. At increasing coverage the results indicate metallization via adsorbed layer, which can be related to Mott transition.

This work was supported by the project N<sup>o</sup> 2.14.99 of Russian National Programme “Surface atomic structures” and by the project N<sup>o</sup> 01-02 of Russian Foundation for Basic Research.

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## AMMONIA ADSORPTION ON A PRISMIC ZNO SURFACE

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Ammonia adsorbed oxide surfaces are one of a fundamental chemisorption system and have been studied extensively over the years. Several authors have been investigated chemisorbed ammonia on ZnO [1-3]. As a Lewis base, ammonia adsorbs on surface Lewis acidic sites, i.e. the Zn atoms, through its lone pair [1]. The IR spectroscopic study for ammonia on ZnO powder has shown a absorption band due to the surface hydroxyl group [2], which is formed through decomposition of adsorbed ammonia. Moreover, ammonia on the Zn-terminated ZnO(0001) surface is also deprotonated upon adsorption [3]. In the present study, we have investigated ammonia adsorption on a prismatic ZnO surface, whose surface is composed of equal numbers of O and Zn atoms, by photoemission spectroscopy (PES) and X-ray absorption spectroscopy (XAS) utilizing synchrotron radiation. The experiment was carried out at beamline 2B1 at UVSOR, Institute for Molecular Science, where the light was monochromatized by a grasshopper monochromator. Ammonia was dosed onto the surface which was kept at 100 K.

As ammonia adsorbs on the prismatic ZnO surface, the PES measurements show that the N 1s peak with the tail to the lower binding energy side is developed at the very initial stages of adsorption. The low binding energy tail is ascribed to the decomposed species of ammonia. However, with increasing amount of adsorbed species, the N 1s peak becomes symmetric, and the low binding energy tail is no more observed. This indicates that a majority of adsorbed species is undecomposed ammonia, which is similar to the adsorption behavior of ammonia on the Zn-terminated ZnO(0001) surface [3].

In the XAS measurements, a submonolayer ammonia-covered surface exhibits three resonance peaks at 400, 405 and 425 eV in the N 1s absorption edge. The 405-eV peak is associated with hybridized states between the N np orbitals and the Zn 4sp orbitals. The 425-eV peak is close to the resonance observed for gaseous ammonia [4], and is assigned to the shape resonance. The threshold resonance peak at 400 eV lies very close to the N 1s vacuum level and should be due to the excitation from the N 1s core level to the low lying unoccupied molecular orbitals of 4a<sub>1</sub> and 2e. It is found that the intensity ratio of these three peaks varies as a function of the electric vector of the light, suggesting a tilted adsorption geometry of ammonia on the surface.

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# HIGH-RESOLUTION SURFACE CORE LEVEL SHIFTS AT THE Cu/Ru(0001) INTERFACE

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Copper adsorption on Ru(0001) has been studied by means of high-resolution photoemission surface core level shifts. The Ru 3d<sub>5/2</sub> core level spectra were measured at the Scienta beam line at ASTRID. Experiments were carried out with copper coverages varying from the submonolayer range up to two monolayers of copper.

The clean Ru 3d<sub>5/2</sub> spectra were found to consist of two components with a binding energy (BE) shift of 400 meV. The component with the lowest BE represents the first layer of ruthenium atoms. Adsorption of copper gives rise to core level shifts of the Ru 3d<sub>5/2</sub> peaks. The BE of the Ru 3d<sub>5/2</sub> surface component increases linearly as the Cu coverage increases from 0 ML to 0.7 ML, with a total BE shift of 85 meV. Core level BE shifts are also observed for the Ru 3d<sub>5/2</sub> high BE component with a 60 meV decrease as the Cu coverage increases from 0 ML to 0.2 ML. As the Cu coverage increases from 0.2 ML to 1 ML the BE increases linearly to the value characteristic of the clean Ru 3d<sub>5/2</sub> spectrum. This is attributed to the effect that this component has contributions from both the Ru 3d bulk core level and the Ru 3d copper interface core level. The latter relatively increases in intensity as the coverage is increased from 0 ML to 0.2 ML where after the relative intensity decreases again, as the coverage is further increased.

Cu 2p<sub>3/2</sub> spectra were obtained with a Mg X-ray source. The BE of the Cu 2p<sub>3/2</sub> electrons is found to be constant at Cu coverages below 1 ML while the BE increases with Cu coverages above 1 ML in agreement with the observations of Rodriguez et al. [1]. In the present study we further determined a strictly linear increase of the Cu 2p<sub>3/2</sub> BE with increasing Cu coverage in the 1 ML to 2 ML interval.

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# Thin manganese films on Si(111): chemical reactions and interface electronic structure

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Thin films of magnetic materials, and their interfaces with semiconductor substrates, are interesting study subjects in view of the recent progress in combining semiconductor technology with magnetic layers [1], for example in nonvolatile magnetic data storage devices and other applications. Here we report on a core and valence level photoemission study of the interaction of manganese with Si(111). Manganese layers have received little attention so far, and the formation of thin films and reacted layers such as silicides, as expected in analogy with other 3d transition metals, has not been investigated in photoemission. Data were recorded at the UE56/2 beamlines at the BESSY II facility; clean Si(111) samples were prepared by flashing of fresh wafers, and manganese layers were deposited from a water-cooled MBE cell at deposition rates of about 1 Å per minute, up to coverages of 15 monolayers thickness. The high resolution and flux up to high photon energies permitted the recording of Mn 2p spectra (binding energy about 640 eV) even for the thinnest layers, along with the Si 2p and valence level spectra.

In the deposition of Mn onto Si(111), we identify several phases as evident from the Si 2p spectra in Figure 1. Deposition of Mn at room temperature leads to an attenuation of the silicon signal as expected. This is followed, upon annealing at temperatures of about 300 ° C, by the formation, for thin films, of a (1 x 1) phase in LEED, characterized by a broad doublet; thicker films leads to the formation of a ( $\sqrt{3} \times \sqrt{3}$ ) R 30° phase which has also been seen in STM studies [2]. The Si 2p signal of the clean surface is very similar to that of the reacted layers, in particular the ( $\sqrt{3} \times \sqrt{3}$ ) R 30° phase, where even the S<sub>2</sub> surface core level seems to be present as a shoulder. This absence of chemically shifted components may indicate that chemical shifts are small; on the other hand, RHEED studies [3] have suggested the formation of a layer of clean, i.e. unreacted Si on top of the reacted layer, as was previously found in nickel silicide [4]. Such a reaction path is also suggested from the weakness of the Mn 2p signal; however, the valence level signature of the reacted phases, with their sharp cutoff at the Fermi level, indicate the formation of a metallic silicide, possibly with a clean silicon top layer. These results will be compared with other 3d transition metal interaction with silicon, and interpreted in terms of known reaction models for metal/silicon interaction.

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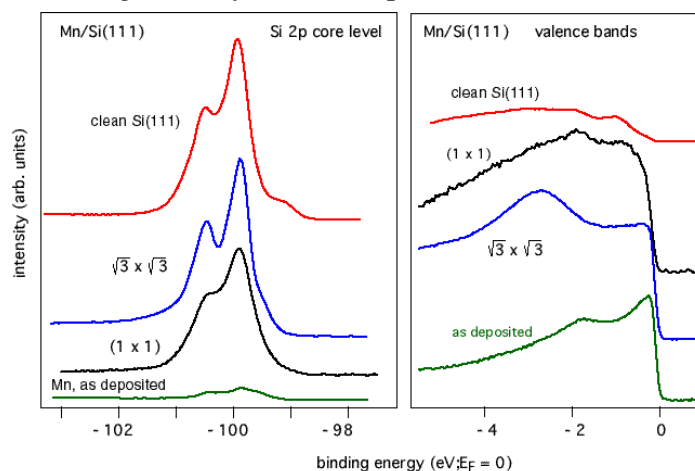


Figure 1: Si 2p and valence band spectra from a series of manganese depositions on Si(111), demonstrating the reaction between the metal and the silicon substrate. The signature of the valence band serves to identify the interface phase as metallic.

## XAFS study of self-organized uniform Ge quantum dots on Si(001)

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GeK XAFS measurements have been performed using the total electron yield and fluorescence yield detection modes for pseudomorphous Ge films deposited on Si(001) substrate *via* molecular beam epitaxy. The samples have been produced by thrice repeating of the growing procedure of Ge films at 300° C separated by deposition of blocking Si layers at 500° C. Two-dimensional pseudomorphous Ge films have grown up to the critical thickness of four monolayers. As a result of the following deposition pyramid-like Ge islands have been grown in Stranski-Krastanov mode. The islands revealing quantum dots (QD) properties [1] are self-organized during the growth in uniform Ge nanostructures with lateral sizes ~ 15nm and height ~ 1.5nm. The effective thickness was changed from four up to ten monolayers for films under the study.

The local microstructure parameters (interatomic distances, Ge coordination numbers) are linked to nanostructure morphology and adequate models are suggested and discussed. It was established that pseudomorphous 4-monolayer Ge films contain 50% of Si atoms on the average. Pyramid-like, pure Ge islands formed in the Stranski-Krastanov growth are characterized by the interatomic Ge-Ge distances of 2.41Å (by 0.04 Å less than in bulk Ge) and the Ge-Si distances of 2.37Å. The values of interatomic distances obtained within the limits of experimental error ( $\pm 0.01\text{Å}$ ) coincide with interatomic bond lengths calculated by valence force field (VFF) method and allowed to understand previous capacitance spectroscopy results. It was revealed that the pure Ge nanoclusters are covered by a 1-2 - monolayer film with admixture on the average of a 50% Si atom impurity from blocking Si layers.

Financial support from the Russian State Scientific and Engineering Program on Physics of Surface Atomic Structures (grant 1-14-99) is greatly appreciated.

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# HIGH-RESOLUTION PHOTOEMISSION AND NEXAFS STUDIES OF METAL-ORGANIC INTERFACES

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The interface between an inorganic substrate and the organic thin films plays a key role in the improvement of organic-based devices since it not only determines the structure and morphology of the organic film and hence its properties but it also strongly influences the electric and optical processes that occur at this interface (e.g., charge injection, quenching of optical transitions) [1]. Our present study is concerned with a detailed understanding of such interfaces for the PTCDA/Ag model system. Using the high-brilliance undulator radiation at the BESSY-II U49/1-PGM beamline we could drastically improve the spectroscopic details obtained so far.

The comparison of the photoemission and x-ray absorption data recorded for PTCDA mono- and multilayers yields new information on the electronic properties of organic thin films and on the molecule-substrate interactions at the metal-organic interface. From high-resolution NEXAFS spectra several new observations can be made: (a) The spectra contain a wealth of fine-structure which is partly due to hitherto unknown electronic transitions and partly to vibrational coupling. (b) The monolayer data show drastic changes compared to the multilayer spectrum which can only be explained by a covalent coupling between Ag and PTCDA. (c) The comparison between the monolayer data taken at 70° and those taken at 0° proves that the molecules are completely coplanar to the surface. (d) The suppression of the first resonance in the monolayer spectra (compared to the multilayer spectrum) is clearly due to the chemical bonding that involves particularly the former LUMO and is accompanied by the appearance of a new structure just below the Fermi edge as seen in photoemission. Since the Fermi level apparently cuts through this bonding orbital one can consider this adsorbate as metallic. (e) The monolayer structures are much broader and display a different fine structure since the bonding to the substrate considerably increases the lifetime broadening of the involved levels which is observed here for such systems for the first time. Similar results have been obtained in photoemission.

Compared to previous XPS experiments of PTCDA multilayers, the now available fine structure clearly reflects several distinct shake-up satellites. The monolayer data look completely different. The shift of the main peak is understandable as arising from bonding to and screening by the substrate. Less clear is the splitting of the main peak which probably arises from a stronger involvement of some of the aromatic carbon atoms in the bonding, but this needs further consideration. Also unclear at present is the appearance of three instead of two smaller peaks at higher BE. Further evaluation and perhaps calculations will clarify the situation. (supported by BMBF, project 05 SF8 WWA 7)

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# Mg-adsorbed on Si(100)2x1 surfaces

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The atomic structure of the Mg/Si(100)-2x2 and -2x3 surfaces has been investigated by using high-resolution photoelectron spectroscopy. The surface were measured at normal emission angle at several photon energies as shown in Fig.1(a) and (b). These spectra were fitted using spin-orbit splitting Voigt function. As seen from the fitting result in Fig.1(c) and (d), the two spectra measured from both surfaces at photon energy of 130eV were reproduced with bulk, two surface components and one second layer component, respectively. The Mg 2p core level spectra showed to be consisted of single component. It seems that these fitting results support a structural model suggested by P. Hunchison *et.al*[1] from STM study.

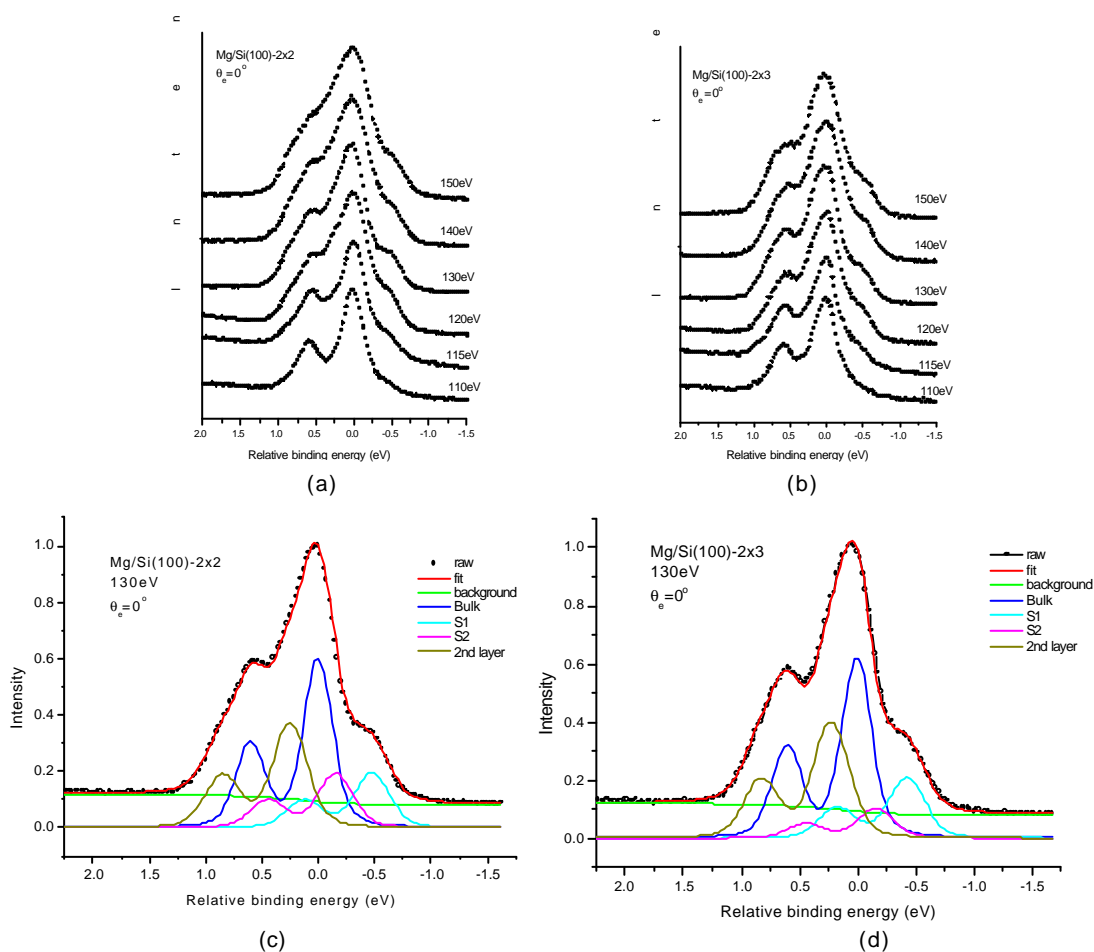


Figure 1. A set of Si 2p core-level spectra taken from the (a) Mg/Si(100)-2x2 and (b)-2x3 surface obtained at various photon energies. (c) and (d) shows the fitting results for the Si 2p core-level spectra taken at photon energy of 130eV at normal emission.

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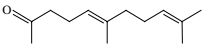
# An adsorption study of Geranyl Acetone on Si(111)7x7 by Valence Band Photoemission and Scanning Tunneling Microscopy

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The connection of organic molecules on semiconductor surfaces is a key problem in a number of advanced technologies such as molecular nanotechniques, nano-sensors and biochips. The first step of such a study implies the adsorption of a polyfunctional molecule, which might have, at the occurrence, one functional group for the surface adsorption, and the other one(s) for further reactions. We present here a test study of adsorption of a polyfunctional molecule, the geranyl-acetone (C<sub>13</sub>H<sub>22</sub>O, ) , which is characterized by two double bonds and a ketone, all of three rich enough in electrons to interact with Si(111)7x7. We performed this study by temperature and coverage dependent valence band synchrotron radiation photoemission and Scanning Tunneling Microscopy (STM). The use of these combined techniques allows us to infer that the molecule does not fragment in any part, as it is for instance the case for acetone on the same surface<sup>1</sup>. Furthermore, the carbonyl group is more reactive than the double bonds with respect to the surface, and as a function of coverage we observe an interaction between adsorbate molecules, a sign that the molecule-molecule interaction is stronger than the carbonyl-surface interaction. The molecules are observed to adsorb preferentially on Si rest atoms, although the Si adatoms are modified by the molecular adsorption through a charge transfer from the adatoms to the rest atoms.

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## A Photon-Stimulated Desorption Approach to Benzene/ Si(111)7x7 Low-Temperature Transitions

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Benzene adsorption on Si(111)7x7 has been under debate due to its peculiar temperature-dependent adsorption states, being physisorbed at temperatures as low as 40 K and turning to a chemisorbed state when the temperature increases above 100 K[1]. We found out that those two adsorption states also show a very different behaviour with respect to the photodesorption process, being the chemisorption state hardly affected by a selective energy irradiation, while the D<sup>+</sup> photodesorption yield is much higher for the physisorbed benzene. We decided, then, to use the photodesorption process as an indication of the benzene state transition. In particular, we performed two types of experiments, one following the D<sup>+</sup> yield at a given temperature as a function of exposure and the other one at a given exposure as a function of temperature.

The first type of experiment is fundamental to determine which exposure range corresponds to a physisorbed state and above which limit we approach the multilayer regime. We found that the D<sup>+</sup> yield curve clearly changes slope for an exposure higher than 0.15 L, that we considered the exposure limit to get a physisorbed state. On the basis of this finding we performed a few sets of experiments at different benzene exposures as a function of temperature. In particular we investigated the D<sup>+</sup> yield at 0.1 L and 0.6 L. Both curves show a yield decrease, though for different temperatures. The physisorbed state shows a change of slope starting at 110 K and the multilayer at 150K. We attribute those two changes of slopes to a transition to a chemisorption state in the first case and to the multilayer desorption in the second one. In order to make sure that the processes are really of a different nature, we compared the D<sup>+</sup> yield to the C1s yield in the same temperature ranges, since a transition to a chemisorption state would not affect the C1s yield. We observe a C1s yield decrease in the same energy ranges as for the D<sup>+</sup> yield for the multilayer and a constant C1s yield as a function of temperature when exposing the silicon surface to 0.1 L. Therefore, we can conclude that we observe a benzene physisorption to chemisorption transition in the temperature range 110-140 K, and a multilayer desorption in the range 150-170 K. We can also assume that the first layer on the silicon surface undergoes a transition from a physisorbed to a chemisorbed state, in the case of multilayer as well, though it is masked by the presence of the layers on top, which eventually desorb for higher temperatures.

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# PHOTOELECTRON DIFFRACTION STUDY OF THE Cs ORDERED LAYERS ON GaAs(110)

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The intrinsic simple nature of alkali metals, together with the absence of surface states in the gap of the III-V surfaces (GaP excluded), candidates their interaction with III-V semiconductor surfaces to be considered as model systems to extract general information on low dimensional systems and related nanostructures. STM[1] and LEED studies[2] found on Cs/GaAs(110) system that the initial formation of Cs zigzag chains is followed, with increasing the coverage, by a two-dimensional overlayer consisting in a c(4x4) superstructure. The electronic structure of Cs/GaAs(110) has been studied extensively by all the spectroscopic techniques available but fundamental aspects, like charge transfer and onset of metallicity, are still under debate. Some calculations[3,4] indicate that the Cs-substrate interaction is dominated by Cs-As bond, other by Cs-Ga bond. A Hubbard model has been also proposed to explain the non-metallic behaviour of the 1ML Cs/GaAs. The lack of structural determination for the system is the major problem for the understanding of this system. Photoelectron Diffraction is particularly suitable because it allows the direct determination of multiple adsorption sites using the chemical shift resolved in high resolution core level photoemission measurements. We performed Photoelectron Diffraction measurements at low kinetic energies[5] on Cs/GaAs(110), at different stages of the interface formation at the core level Cs 4d, As 3d and of Ga 3d in order to shed light on structural details in the two ordered systems (chains and c(4x4)). We found that the PhD modulations of the cation substrate core level present strong changes induced by the Cs deposition, more pronounced at the symmetry directions, while the anion PhD signal is much less perturbed with respect to the clean signal. This finding should confirm the preferential adsorption on the cation site. The analysis of the structural model will be discussed.

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# Intra-atomic versus interatomic process in resonant Auger spectra at the Ti $L_{2,3}$ edges in rutile

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The chemical nature and environment of an element often manifest themselves through the occurrence of specific electronic transitions. In ionocovalent compounds, the severely depleted valence population of the cations favors a possible interatomic core hole Auger decay. Furthermore, it has been evidenced recently that core level electrons of neighboring atoms can be direct actors in the resonant photoemission process of the excited atom which can have applications as a probe of the hybridization with the external orbitals of neighboring atoms [1]. In transition metal oxides, the occurrence of interatomic transitions in Auger decays involving valence electron has suggested to make use of them to determine the surface stoichiometry. In  $TiO_2$ , the stoichiometry has been shown to be directly related to the ratio of the two components of the Ti  $L_{2,3}M_{2,3}V$  Auger transition [2]. Due to its appearance when the metal is oxidized and its increase in intensity upon increasing the oxidation state of the metal, the low kinetic energy component is assigned to a so-called "interatomic LMV(O)" decay, while the other component is associated to an "intra-atomic LMV(Ti)" process (V(Ti) and V(O) refer to Ti and O contributions to the oxide valence band).

In this work, the two components of the Ti  $L_{2,3}M_{2,3}V$  Auger transition recorded on a stoichiometric rutile crystal are identified as  $L_2M_{2,3}V$  and  $L_3M_{2,3}V$  contributions. This assignment is evidenced by concordant data relative to resonances of the LMV decay at the Ti  $L_{2,3}$  thresholds and to Auger emission recorded in coincidence with the  $2p_{1/2}$  and  $2p_{3/2}$  photoemission at a photon energy far above the Ti  $L_{2,3}$  edges. The  $L_3M_{2,3}V$  transition is shown to follow either the direct photoexcitation of a  $2p_{3/2}$  electron or the fast Coster-Kronig decay of a  $2p_{1/2}$  photohole. Although specific LMV contributions related to valence orbitals are identified, the long-suggested dual description of the  $L_{2,3}M_{2,3}V$  Auger line as intra-atomic and interatomic transitions is discarded.

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## **Role of the gold self-surfactant effect on the growth mode and the morphology of Fe/Au(001) magnetic thin films.**

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During the last decade, a great amount of attention has been given to understanding the role played by atomic process in the growth of thin films. The simple and fundamental theories of epitaxial growth have been modified and extended to include new phenomena: preferential nucleation, anisotropy surface diffusion, segregation, place exchange at the interface...The former phenomenon can results in the formation during the growth of a surface alloy or a deposited layer encapsulated by a layer of substrate atoms. The presence of such floating layer is of particular interest since it can play a self-surfactant role and lead to significant modification of the epitaxy[1] and then of the magnetic properties in magnetic thin films.

The Fe/Au(001) system is a good candidate to investigate the role of atomic process in the growth mode and the correlation between structure of thin films and magnetism. It is well know that the gold plays the role of self-surfactant during the growth of Fe/Au(001) thin films[2], leading to a segregated Au layer and a buried epitaxial Fe bcc films. In spite of an important number of studies [3,4,5], little is known on how this action occurs and the way in which the self-surfactant role of the gold substrate makes the system grow epitaxially.

We report a combined high-resolution photoemission and spectromicroscopy study of the self-surfactant effect in the growth of Fe/Au(100). Core level photoemission measurements have confirmed the formation of AuFe surface alloy in the Fe submonolayer range. For higher coverage up to 15ML, a significant signal from the Au4f has been measured, confirming the presence of a gold floating layer. The analysis of the Au4f line shapes allows us to conclude to the presence of at least two different kinds of environment for gold atoms in the floating layer. This can correspond to a mixing of different domains for gold: pure layer (adatom or embedded), a surface alloy or islands (2D or 3D phases).

Spectromicroscopy measurements have shown clearly and then confirm the chemical non-homogeneity of the growth of Fe/Au. For low coverage, the growth proceeds by the segregation of small gold islands (<500nm). For higher coverage, the size of the islands increases while their density decreases. From these results, we can conclude that the gold atoms segregate via an exchange mechanism leading to the formation of a AuFe surface alloy. This mechanism has been already shown for low coverage. However, the reduced mobility of gold atoms at room temperature, does not allow a complete segregation and limits then the self-surfactant effect.

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## Lateral effects in the Cu/GaS<sub>x</sub>Se<sub>1-x</sub> interfaces formation

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The Cu/ GaS<sub>x</sub>Se<sub>1-x</sub> interfaces are investigated by the mean of a synchrotron-based scanning photoelectron spectromicroscope (SPEM) of the Schwarzschild optics type. In particular we present the results for the case  $x=0$  and  $x=0.4$ . As compared to conventional X-ray photoemission spectroscopy (XPS), with spectromicroscopy we can provide spatially resolved chemical information. All the data presented here have been acquired at the Spectromicroscopy beamline in ELETTRA.

Using the combined study of images recorded with the energy tuned at different values and core level spectra taken along the interfaces, we analyzed the differences between the interfaces, due to changed surface reactivity of the two substrates. By taking microimages in all the systems tuned on the Ga 3d and on the Se 3d core levels we can find out the presence of an intermediate zone in proximity of the Cu overlayer edge where reacted chemical species are visible for a well defined coverage. In addition to the two components that correspond to bulk and surface atoms, the detailed analysis of Ga 3d photoemission spectra reveals the presence of a metallic and reacted Ga components with different energetic positions. The reaction takes place in the first stages of the interfaces formation and the lateral resolution of the technique allows to monitor its spatial distribution.

# X-ray photoelectron and absorption spectra of fragments from NH<sub>3</sub>/Cu(110) induced by soft x-ray irradiation

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We have studied fragments from NH<sub>3</sub> molecules adsorbed on Cu(110) induced by soft x-ray irradiation using x-ray photoelectron spectroscopy (XPS) and x-ray absorption spectroscopy (XAS) in combination with theoretical calculations. The soft x-ray induced dissociation of NH<sub>3</sub> adsorbed on Cu(110) leads to desorption of H<sup>+</sup> ions and H<sup>0</sup> neutral atoms leaving the NH<sub>x</sub> fragments on the surface [1,2]. Characterization of the NH<sub>x</sub> is significant for understanding the dominant dissociation process by soft x-ray irradiation.

The experiments were carried out on the surface end-station at undulator beam line I511 at MAX-lab. The analyzer chamber at the end-station is equipped with a spherical electron spectrometer (SCIENTA SES-200) for XPS and a partial electron yield detector for XAS. The Cu(110) crystal was cleaned by cycles of Argon ion sputtering and annealing to 800 K. NH<sub>3</sub> was adsorbed at 90 K and annealed to 140 K for 10 min to obtain only the chemisorbed NH<sub>3</sub>.

Figure 1 shows the N 1s photoelectron spectrum before and after soft x-ray irradiation. There are two peaks: the higher-energy peak is assigned to the chemisorbed NH<sub>3</sub> in both spectra and the lower-energy peak arising from the irradiation is assigned to NH<sub>x</sub> fragments. In the photoabsorption spectrum at the N K edge, the fine structure of the NH<sub>x</sub> was also observed. We will present the assignment and the electronic structure of the NH<sub>x</sub> based on the theoretical calculations.

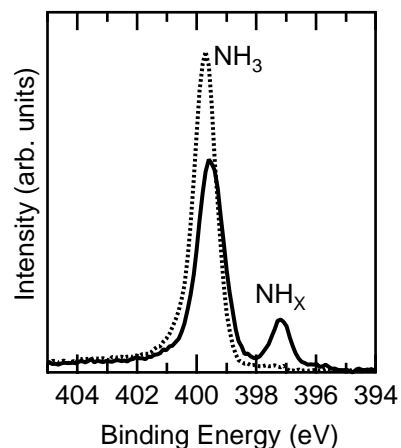


Figure 1. N 1s photoelectron spectra of NH<sub>3</sub> on Cu(110) before irradiation (dotted line) and after (solid line).

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# Modification of the surface states induced by Ga deposition on InAs(001)

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With growing technological use of group III-V compound semiconductor heterostructures in advanced applications, an understanding of the physical properties of these systems is important. In this work we have used in-situ ultraviolet and synchrotron radiation photoelectron spectroscopy to investigate the electronic structure of Ga deposited on InAs(001) surfaces. The surface states induced by Ga deposition on the InAs(001) 2x4 reconstructed surface, seen in Fig.1, are detected near the valence band edge, and are similar to surface states of the InAs(001) 4x2 reconstructed surface. In contrast, upon Ga deposition on the InAs(001) 4x2 reconstructed surface, no prominent surface state appears near the valence band edge. The results obtained from analyses of the core-level spectra and reflection high-energy electron diffraction indicate that the presence of Ga deposition-induced surface states are related to the group-III (In or Ga) atom-stabilized surface reconstruction.

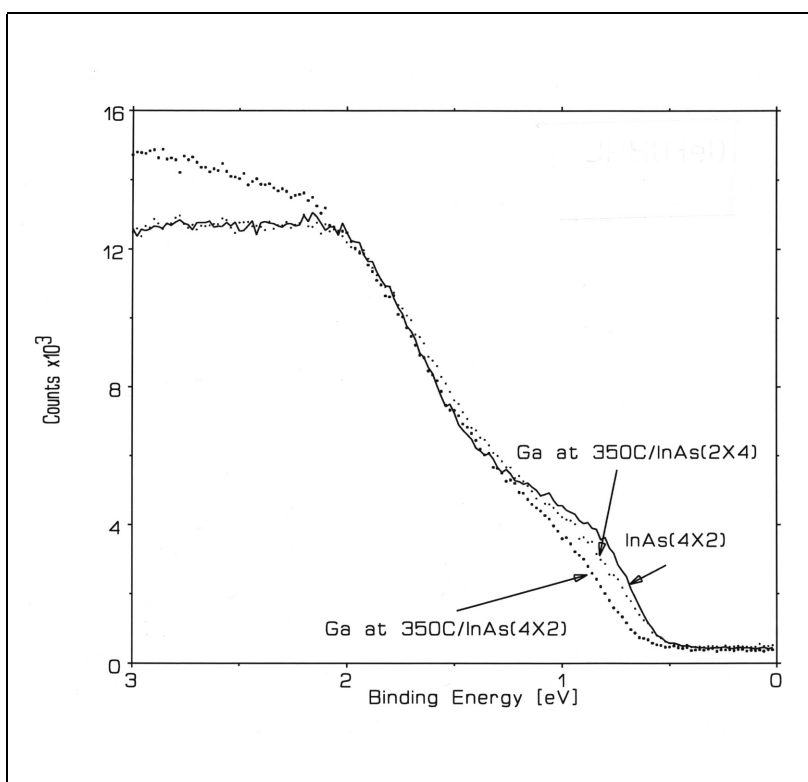


Figure 1: Valence band spectra of Ga deposited on InAs(001) 2x4 and 4x2 reconstructed surfaces and a clean InAs(001) 4x2 surface.

# Band discontinuity of heterojunction GaAs/AlAs studied by Synchrotron Radiation *in situ* photoemission spectroscopy

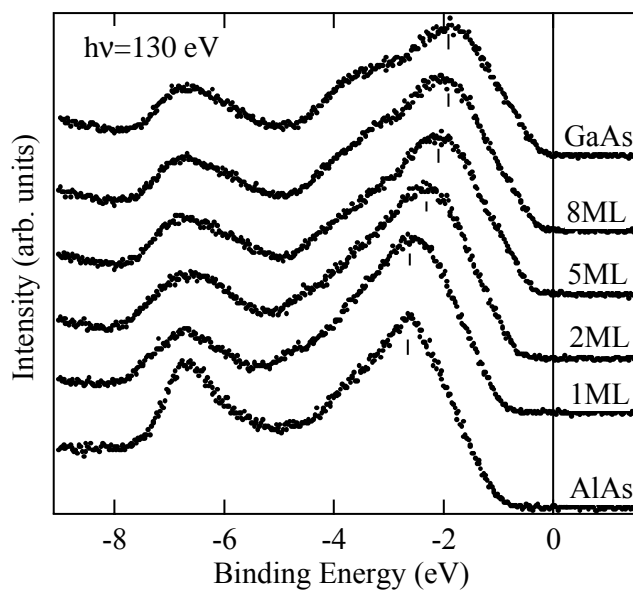
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A photoemission system combined with molecular beam epitaxy (MBE), called '*in situ* photoemission', enables the new research field of nanostructures [1]. III-V semiconductor heterojunctions, especially GaAs/AlAs, with small lattice-constant mismatch have high potential for device applications using energy-band discontinuity. In order to investigate the valence-band discontinuity, we performed *in situ* photoemission spectroscopy (PES) at BL-1C, Photon Factory, KEK, Japan.

The GaAs layer thickness dependence of GaAs/AlAs shows a continuous peak shift of the valence-band maximum as shown in Fig. 1. The peaks in each of the GaAs and AlAs spectra has about 0.4 eV binding energy difference [2] and the spectrum of GaAs with 8 ML (~2 nm) thickness shows almost the same feature as bulk GaAs, which means that 8 ML GaAs is enough for probing only the GaAs layer in the GaAs/AlAs heterostructure. For thickness less than 8 ML, PES spectra behave as Al<sub>1-x</sub>Ga<sub>x</sub>As with respect to the concentration x dependence. Thus we conclude that GaAs/AlAs system behaves as Al<sub>1-x</sub>Ga<sub>x</sub>As in thin limit, which is the same behavior as GaAs and AlAs digital growth.



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Figure 1. GaAs layer thickness dependence in the valence-band region.



# Quantum-well states in ultrathin Ag(111) films deposited onto H-passivated Si(111)-(1x1) surfaces.

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During the last years, the study of low-dimensional structures has attracted considerable interest because of spatial confinement of electrons in thin films results in discrete quantum-well states (QWS). This phenomenon has been found in semiconductors, in two-dimensional metal overlayers, and recently, in quasi-zero-dimensional metallic quantum dots. In semiconductor layer systems, these effects are well known, and it has been already used in electronic devices. However, the observation of quantization effects in metallic layers, has been restricted to a few systems. In this respect, thin films of Ag metals have attracted strong interest due to the nearly free-electron characteristics of the *sp*-like bands over large regions of the Brillouin zone. Ag *sp* QWS have been widely observed in thin Ag films deposited over several metallic substrates[1]. However, observation of confinement effects on silver films deposited over semiconductor substrates has been restricted to a few systems[2]. Weak peaks associated to QWS have been observed by Wachs et al[2] in the photoemission spectra of 0-17 monolayers (ML) Ag films deposited on Si(111)-(7x7). The weakness of the QWS observed by these authors could be associated to the formation of non-uniform thickness Ag films, suggesting that an improvement of Ag deposition conditions and silicon substrate preparation, could play a key role for the observation of well-defined QWS in thin Ag films deposited on silicon substrates.

By this reason, in this work thin silver films have been deposited in ultra-high-vacuum at room temperature onto H-passivated Si(111)-(1x1) substrates, and subsequently annealed at 300°C to enhance the film uniformity. By such a procedure, Ag grows in a quasi-layer-by-layer mode, forming islands much thinner than those on the non-passivated substrate[3]. In such a way, an abrupt non-reactive Ag/Si interface is formed, and high-quality thin Ag films of 6-13ML have been obtained.

The quality of the silver films has been probed by angle-resolved photoemission spectroscopy. Well-defined Ag *sp* QWS have been observed at discrete energies between 0.5–2eV bellow the Fermi level. The energy dispersion of the QWS as a function of the parallel wave vector has been measured along the  $\bar{\Gamma}\bar{K}$  and  $\bar{\Gamma}\bar{M}$  symmetry directions, showing a parabolic behavior with in-plane effective mass of 0.38-0.46. Varying the photon energy, no dispersion has been found as a function of the perpendicular wave vector. On the other hand, the binding energy dependence of the QWS as a function of Ag film thickness has been analyzed in the workframe of the phase accumulation model[4]. A good agreement between experimental data and the above mentioned model is obtained for the Ag/H/Si(111)-(1x1) system.

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# Ferromagnetic properties of low temperature early stage deposition of Fe/Si(111)-7x7 interface

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Magnetic thin films have shown recently phenomenology that cannot be observed in bulk materials. Growth conditions and substrate morphology characteristics can lead to surprising magnetic behaviours. It is well known that the substrate has substantial influence on the structure, growth mode and magnetic properties of ultrathin overlayers<sup>1</sup>; in particular one of the problems in the growth of the magnetic structures on semiconductors substrates is the intermixing of the overlayer and substrate elements. Growing magnetic overlayers at low temperature, and hence retarding the diffusion (of the overlayer) and/or the segregation (of the substrate), might provide a possible solution to this problem.

The debate still passionate many researchers and also recently the Fe/Si(100) and Fe/Si(111) interfaces have been investigated with different techniques to study the nature of the iron silicides<sup>5</sup> related with their magnetic properties<sup>2-4</sup>. Here, we report a low temperature epitaxial growth of Fe films on Si(111)-7x7, in the thickness range of 1.5ML, by means of photoelectron spectroscopy, X-ray magnetic circular absorption and photoemission core-levels spectroscopy. Our measurements show a magnetic interface formation in spite of the low density of iron on silicon.

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## Silicide islands at the Au/Si(111)-H interface: the role of H passivation

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The high degree of order and passivation of the H/Si(111)-7x7 system, prepared by atomic hydrogen exposure, makes it an ideal prototype for understanding chemisorption phenomena <sup>1</sup>. Nonetheless metal-silicon interfaces are of crucial importance for the Si-based technology, in particular the gold-silicon interface has been extensively investigated by several different techniques and models to improve Schottky barriers and Ohmic contacts fabrication <sup>2-4</sup>. The aim of this paper is to elucidate the reaction at the Au/Si(111)-H interface as a function of the annealing temperature: the sample is cleaned by chemical etching, protected by chemical growth of a thin oxide film (which is desorbed in-situ) and exposed to atomic hydrogen. After deposition of gold we have concentrated our attention on Si2p and Au4f core levels as a function of the temperature up to 800°C by means of PES and Scanning Photoemission Microscopy. Our results show the presence of silicide islands that have been analysed from the point of view of chemical and electronic properties.

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# ADSORPTION BEHAVIOUR OF THIOPHENE ON NOBLE METAL SURFACES

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The interaction of thiophene with metal surfaces is of interest from the viewpoint of fundamental understanding of hydrodesulfurization process in the petrochemical industry. In this work we have studied the structures of thiophene adsorbate on noble metal surfaces (Au, Ag and Cu) with several coverages, from sub-monolayer to multilayer, by mainly C *K*-edge and S *K*-edge near edge x-ray absorption fine structure (NEXAFS).

All NEXAFS experiments were carried out at soft x-ray beamline 7A and 11B of Photon Factory (KEK-PF, Tsukuba, Japan). The measurements were performed in ultrahigh vacuum (UHV) chambers connected to the beamlines. Metal substrates were cleaned by the cycles of Ar<sup>+</sup> sputtering and annealing. After cleaning, the substrates were exposed to gaseous thiophene at low temperatures.

In the sub-monolayer region, the incident angle dependence of a peak assigned to 1s <sup>\*</sup><sub>1</sub> peak of C *K*-NEXAFS spectra indicated that thiophene adsorbs with a flat-lying configuration on all the metal surfaces.

Figure 1 shows S *K*-edge NEXAFS spectra of a multilayer of thiophene adsorbed on Au(111) with different x-ray incident angles. There is the incident-angle dependence of spectrum, which means that thiophene molecules in the multilayer on Au(111) were adsorbed with a standing configuration. Figure 2 shows S *K*-edge NEXAFS of a thiophene multilayer on Cu(100). There is little polarization dependence of spectra. We could conclude that the absence of polarized dependence indicates the orientation of thiophene multilayer on Cu(100) is random. The result for Ag(111) is the same as that of Cu(100).

The significant difference in molecular orientation of multilayer between Au(111) and other metal surfaces (Ag and Cu) might be attributed to the difference in the structure of the first-layer in multilayer. In the case of Cu(111) and Ag(111), there has been some studies reporting about so-called compressed monolayer of thiophene, where the monolayer adopts a standing configuration, however there is no report on Au(111). Now we are investigating the structure of adsorbed thiophene in the saturated monolayer on each metal surface, and the detailed results will be presented in the Conference.

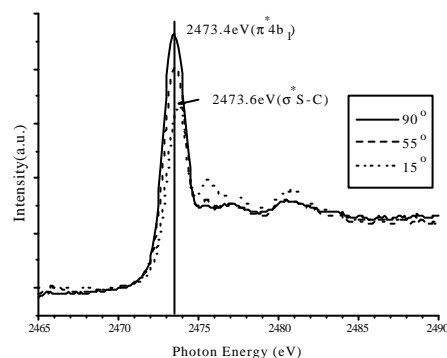


Figure 1: S *K*-NEXAFS of Thiophene Multilayer on Au(111); The incident-angle dependence shows a standing configuration of molecules.

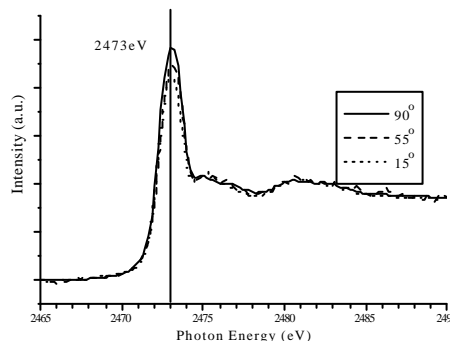


Figure 2: S *K*-NEXAFS of Thiophene Multilayer on Cu(100); No incident-angle dependence is observed.

## **A BEAMLINE FOR PHOTOELECTRON-MICROSCOPY AT THE SWISS LIGHT SOURCE (SLS)**

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We describe the "Surface/Interface: Microscopy" (SIM) beamline currently under construction at the Paul Scherrer Institute. This beamline will use a commercial photoemission electron microscope to study the electronic and magnetic structure of a variety of materials. Its photon energy range will be 94 to 2000eV. It uses elliptical undulators allowing full control of the light polarization (linear 0-360°, circular right- or left-handed).

In order to allow for time resolved measurements (~1ms resolution) we developed a new scheme allowing to switch the photon helicity optically without interference with the storage ring. We use two identical elliptical undulators located behind each other in the same straight section. They can produce light with opposite helicities. These two sources are separated by introducing a small static parallel offset in the electron orbit. Switching between the two opposite helicities takes place at the horizontal focus behind the monochromator. The X-rays are brought to overlap by moving the sample slightly out of focus.

The optical components and the microscope are currently being installed and first test results will be reported. The commercial microscope (25 nm resolution) is adapted to the synchrotron by various upgrades. These include sample cooling ( $T_{\min} \sim 110\text{K}$ ), a separate sample preparation chamber, a control system combining microscope and beamline operation and a computer controlled alignment system. The beamline will be available for user operation in 2002.

# THE TRANSITION FROM AMORPHOUS SILICON OXIDE TO CRYSTALLINE SILICON STUDIED BY PHOTOELECTRON DIFFRACTION

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Thermally grown SiO<sub>2</sub> was prepared on Si(111) surfaces and was studied by angle-scanned high resolution photoelectron diffraction. The photoemission spectra were recorded for a photon energy of 155 eV at the U49/1-SGM beamline at BESSYII using an hemispherical electron analyzer with an angular acceptance angle of 4°. The electron energy resolution was about 50 meV, the photon energy resolution was set to 80 meV. The photoemission spectra were recorded over 180° azimuth range and 84° polar angle range, each with a constant increment of 2° over the full range. With the energy resolution used, it is possible to resolve four additional and chemically shifted components (Si<sup>1+</sup>, Si<sup>2+</sup>, Si<sup>3+</sup>, and Si<sup>4+</sup>) with the Si bulk signal in a Si 2p photoelectron spectrum. We present data showing the first full 2 $\pi$  photoelectron diffraction data of all oxidation states at the surface.

As an example, Figure 1 displays the experimental diffraction pattern recorded for a clean Si(111) surface and the pattern of the Si<sup>1+</sup> chemically shifted state. The two different patterns reflect the individual local environment for atoms in different oxidation states. We compare the experimental with simulated diffraction patterns obtained for various assumed interface structures. The results within an R-factor analysis indicate horizontally compressed silicon oxide at the interface with a bond length of SiO<sub>2</sub>. Also, while the R-factor analysis was performed for each suboxide separately, structure parameters obtained for common atom bonds of all the suboxides are in good agreement to each other.

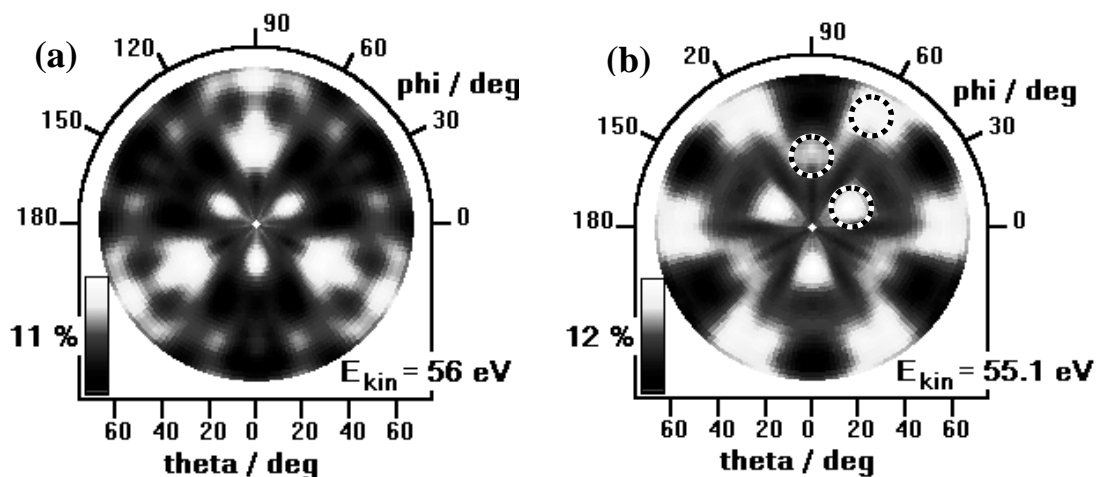


Figure 1: Photoelectron diffraction patterns of silicon surfaces: (a) bulk signal, clean surface (b) Si<sup>1+</sup> chemically shifted state below amorphous silicon oxide

# Photoelectron diffraction study of Si 2p surface-core-level-shift component of Si(001)1x2-Sb

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The structural model of Si(001)2x1-Sb surface has been well established in which Sb dimers occupy a bridge site of Si(001)[1]. However, the origin of a major Si 2p surface-core-level-shift (SCLS) component is not yet certain as appeared in recent experiment[2] and theory[3]. In this report, the SCLS resolved Si 2p photoelectron diffraction (PED) is used to clarify the origin of the SCLS component.

The experiment was carried out on the undulator beamline, BL-13C at KEK-PF, Japan. A home-built PED chamber that equipped a VG-CLAM4 analyzer and a motor controlled sample manipulator was connected to the beamline. A single-domain (SD) Si(001)2x1 substrate was made by a DC heating at ~1520 K of an well-oriented Si wafer. Sb was deposited onto the SD 2x1 surface at room temperature. A subsequent annealing at ~830 K for 1 min resulted in the change in LEED pattern from 2x1 to 1x2. Si 2p photoelectron spectra were measured for the 1x2 sample at a surface-sensitive photon energy of 136 eV. The origin-unknown dominant SCLS component was found in the Si 2p spectra at a binding energy, 0.6 eV smaller than the bulk component. SCLS Si 2p PED patterns were obtained from the sets of azimuthal-angle-scanned Si 2p spectra.

The simulation of the PED patterns were made using MSCD program[4] for the assignments of Padova et al.[2] and Cho et al. [3] In the former assignment, the SCLS component is ascribed to the first layer Si together with some second layer Si. In the later, it is ascribed to some of the second layer Si atoms. The simulation for the former assignment showed close similarity to the experiment while it was not the case for the later. This suggests that the SCLS component mainly originates from the first layer Si atoms.

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## Photoelectron diffraction study of ethylene adsorption on Si(001)

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Ethylene adsorption on Si(001) surface is a model system of pi-bonded hydrocarbon adsorption on Si(001) and there were a pioneering work by Yoshinobu et al.[1] and a structural study by Terborg et al.[2] In this work, C 1s photoelectron diffraction (PED) patterns were measured and compared with results of simulation with different coverage of ethylene molecules adsorbed on Si dimers.

The experiment was carried out on the undulator beamline, BL-13C at KEK-PF, Japan. A home-built PED chamber that equipped a VG-CLAM4 analyzer and a motor controlled sample manipulator was connected to the beamline. A single-domain (SD) Si(001)2x1 substrate was made by a DC heating at ~1520 K of an well-oriented Si wafer. 10 L ethylene exposure was made onto the RT Si(001)2x1 substrate. The photon energy used for the PED measurement was 386 eV. The simulation of the PED patterns was made using MSCD program[3] with model clusters of adsorbed ethylene and 6 Si layers including dimers.

Simulational patterns for a full-coverage model cluster in which ethylene molecule adsorbs every dimer-site on SD Si(001)2x1 showed unsatisfactory agreement with experiment even for the previously optimized geometry[2]. Simulational patterns for the full-coverage model cluster in which a distortion of adsorbate complex[4] is included showed no improvement. Simulational patterns for a model cluster in which an isolated ethylene molecule is present on a dimer-site agree better with experiment. Further detailed simulation with different degrees of ethylene coverage showed that ethylene molecules are present on every other dimer-sites along the dimer-row. These results are consistent with recent coverage-dependent high-resolution photoemission study[5] and STM study[6].

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## Valence-band resonant photoemission of $\text{Cr}_2\text{O}_3$

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Resonant photoemission measurements evidence the interference effects occurring between the direct photoemission channel and the Auger-like de-excitation channel opened up by the photon excitation of a core level. Intensity modulations of the photoemission cross-section are measured as a consequence. Similar modulations were also reported for the satellite features of the main photoemission line of transition metals[1,2]. In this case, however, the direct and the recombining channels share the singly ionised two-hole final state. The intensity of the resonant photoemission signal also reflects the availability of the empty states involved in the hole decay process.

This study presents valence-band resonant photoemission data on  $\text{Cr}_2\text{O}_3$  at the metal  $L_3$  absorption edge. The density of states near the Fermi level is modified with respect to the metal case by the oxygen. We observed a high interference effect on the Cr  $3d$  main line, in partial agreement with previous results on Cr metal[2]. However, the binding energy position of the Cr  $3d$  line increases discontinuously in correspondence of the absorption from  $2p$  core states to the empty states of the ligand field atomic multiplet[3].

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## ANGLE-SCANNED PHOTOELECTRON DIFFRACTION: FROM CLEAN SURFACES TO COMPLEX ADSORPTION SYSTEMS

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Recent selected applications of low-energy, angle-scanned photoelectron diffraction (PED) for surface structural determination are described, with the aim of highlighting the advantages of the angle-scanning approach.

In the first experiment, we used surface-core-level shift PED for the determination of the clean Rh(110) surface layer relaxation. The bulk and surface components of the Rh  $3d_{5/2}$  core level were measured as a function of the azimuthal angle in a high resolution photoemission experiment. Both components display strong modulations with a periodicity reflecting the symmetry of the crystal. The experimental PED data have been analyzed by comparison with multiple-scattering cluster calculated curves. A preliminary evaluation yields relaxation values in good accord with previous LEED-IV determinations.

In the second experiment, a system lacking of long-range order is examined, namely the saturation layer formed by nitrogen monoxide on Rh(100) at 123 K. We show that this phase is locally well-ordered, yielding N  $1s$  PED curves identical to the well ordered  $p(4 \times 2)$ -NO phase produced by heating the system to 390 K, proving that the two phases have the same local geometry. By multiple scattering cluster calculations the adsorption geometry model and structural parameters have been determined.

The last example is a recent chemical shift PED study of the  $c(4 \times 2)$  phase of carbon monoxide on Pt(111). This is a complex system where CO molecules adsorb at different adsorption sites, showing a 0.7 eV chemical shift in the C  $1s$  binding energy. We exploit the capabilities of this technique to yield quantitative information on the local structure around inequivalent atoms of the same species coadsorbed on the surface, by measuring and simulating the angular dependence of both chemically shifted C  $1s$  core levels.