## Poster Sessions

measuring the variations of lattice constants of iso-strained substrate layers at different penetration depths. This method is now applied to investigate the strain field of quantum dots nano-structures of FeSi2/Si. Choosing one secondary diffracted beam along the interface (parallel to the surface of the substrate) between the quantum dots and the Si substrate, the diffraction images of the secondary diffraction, recorded on a charge coupled device (CCD), provide the information of the interfacial structures. The three-dimensional strain and a theoretical calculation of X-ray scattering from quantum dots at the Bragg-surface diffraction geometry based on the dynamical theory will be also reported.

Keywords: FeSi<sub>2</sub>, interface, diffraction

## P12.01.12

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# Oxygen-induced D03-sublattice disorder at the Fe<sub>3</sub>Al(110) surface

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Alloys of Fe and Al form promising materials for high-temperature light-weight replacements of steel [1]. However, for their use in real applications, the understanding and control of the oxidation behaviour is crucial [2]. Here, the atomic structures of the clean and oxidized Fe<sub>3</sub>Al(110) surface are studied by in situ surface X-ray diffraction using synchrotron radiation. The results for the clean surface demonstrate that the topmost atomic layer exhibits in-plane B2 order, with a D03 bulk beneath it. Upon oxidation at 10<sup>-6</sup> mbar of molecular oxygen at a temperature of 573 K, the D03 long-range order in the near-surface region disappears completely, without affecting the surface roughness nor the crystallinity. At the same time, a smooth 8.4(3)  $\cong$  AA  $\cong$  thin aluminium-oxide layer is formed on the surface, as concluded by complementary X-ray reflectivity and Auger Electron Spectroscopy measurements. These results can be understood by preferential surface seggregation in combination with a high affinity of Al for oxygen. These findings are very important for real applications of iron-aluminides, since their physical properties depend stronly on the composition and the resulting ordering. The present result of oxygen-induced Al-depletion is expected to result in a stronger and less brittle selvedge than the bulk beneath, which has important implications for the processing of these materials.

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Keywords: oxidation, binary metal surfaces, surface X-ray diffraction

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## PTRF-XAFS investigations on the interaction between metal and the oxide support

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Metal-oxide interaction plays an important role in catalysts, sensors, electric devices, optical materials and so on. Single crystal oxide systems are used as model system and a  $TiO_2(110)$  surface is most widely studied. We have investigated Ni on  $TiO_2$  (110) using polarization-dependent total reflection fluorescence X-ray absorption fine structure(TPRF-XAFS) to clarify the real metal-oxide interaction directly. XAFS measurements were carried out at BL9A in Photon Factory. Ni was deposited on the  $TiO_2$  (110) by resistive heating under

UHV conditions. Polarization dependent measurements were carried out in 3 different directions. Ni K-edge XAFS oscillations as shown in Fig. 1 indicated the presence of large number of Ni-O bonds especially in the [11b0] direction in addition to the Ni-Ni interaction. We proposed the cluster structure as depicted in Fig.1d. In this structure Ni atoms in the cluster was arranged in a Ni (110)-like structure parallel to the surface. The one-atomic layer Ni clusters was stabilized by the interaction with oxygen atoms.



Keywords: X-ray absorption fine structure, surface structure, oxide surfaces

## P12.04.14

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#### Total reflection of X-rays due to diffraction

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Total reflection of x-rays due to diffraction. In a popular X-ray diffraction book [1], the diffraction and the reflection are treated as completely different physical phenomena: (1) The diffracted X-rays by the crystal are formed by scattering from all the atoms irradiated by the incident X-rays, but visible light is only reflected by the surface thin layer. (2) Monochromatic X-ray diffraction by a crystal takes place at the Bragg angle, but the visible light reflection takes place at any angle. (3) The reflection by a mirror is about 100 %, and the intensity does not decrease due to the reflection, but the diffracted X-ray intensity is extremely weaker than the incident X-rays. However, I would like to claim that the X-ray diffraction and the X-ray total reflection, which is similar to the visible light specular reflection, are both diffraction phenomena. Takahashi and Nakatani have already claimed this at 1995 [2]. The consequence of the above discussion will be: (1) the total reflection intensity profile is the Darwin profile, which has been pointed out by Ref.[2]; (2) the critical angle of X-ray total reflection can be interpreted from the dynamical theory of X-ray diffraction. The fundamental of X-ray total reflection is important for the practical application of total reflection X-ray fluorescence for sub nanogram analysis [3]. Some applications of the X-ray specular reflection are also presented. References

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Keywords: total reflection X-ray fluorescence, dynamical theory of X-ray diffraction, Darwin profile

## P12.04.15

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### Micro and quick reflectometry with high-energy white synchrotron X-rays

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X-ray reflectivity is sensitive to slight structural changes along the depth of layered materials in the order of sub-nanometers or even smaller. This property is extremely promising for the observation of buried layers and interfaces of multilayered thin films. So far, the method looks at quite wide area (mm<sup>2</sup>~cm<sup>2</sup>) and requires typically 20min~1h for one measurement. Here we report the instrumentation for upgrading the technique to give it a much higher spatial resolution with very quick measurement. The experiment has been done with high-energy white synchrotron beam ranging up to 100 keV, at BL28B2, SPring-8. Parallel small beam of 17micron(H) x 5.5micron(V) has been formed by several pairs of thick blade of tungsten. The data have been taken by a silicon drift detector as X-ray reflection spectra. One can analyze inhomogeneous layered thin films with around 20 micron resolution, and even scanning has become possible. Figure shows the results of the line scan of a patterned sample which has Cu, Cr and Au layer on the same substrate. Further experimental details and results will be presented.

References

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Keywords: grazing incidence, microbeam analysis, energydispersive analysis

## P12.04.16

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#### Melting behavior of substrate-free polystyrene surfaces studied by X-ray reflectivity

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Glass transition, melting and solidification in the surface region of polystyrene (PS) were observed by surface-sensitive X-ray reflectivity (XR). Unlike the studies reported, in which ultrathin layers with several nm thick had been prepared by the spin coating method on flat substrates, we used the surface of bulk PS with several mm thick. The reason why we adopt such a PS surface is to reveal the kinetics and dynamics of glass-forming polymers on the surface without any effect from the substrates. Not a few results on physical properties on thermal behaviors of glass-forming polymer surfaces would severely be affected by the physical and chemical properties of substrates, and by residual solvents. A lump of solventfree PS (glass transition temperature: ca. 373 K) melted on a Si (100) wafer at 450 K in low vacuum for 6 hours was cooled down to the room temperature with a cooling rate of 1 K/min. Then, the PS was removed from the Si to obtain the flat surface of PS with 2 cm X 2 cm in area and 2 mm thick. The surface of PS was found to be extraordinary flat; the root-mean-square roughness of the surface was fitted to be 1 nm by XR measured at room temperature, which was also confirmed by AFM. XR at various temperatures up to 400 K is now undertaken to obtain the temperature dependence of surface roughness, height-height correlation function, and electron density of the novel PS surface.

Keywords: melting, surfaces, X-ray reflectivity

## P12.04.17

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### Time-resolved X-ray reflectivity investigation of lysozyme adsorption at the air-water interface

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X-ray reflection measurements of a globular protein adsorped at the air-water interface was demonstrated using recently developed liquid interface reflectometer at SPring-8. The reflectometer equipped with two-dimensional hybrid pixel array detector, PILATUS,

achieved only 1 sec, having enormous potential for quick measurements. A globular protein, lysozyme (LSZ) was injected into a phosphate buffer solution. The reflectivities shown in Fig.1 were measured under non-equilibrium condition, 4 sec after the protein injection. The time required each measurement was 150 sec. A broad peak observed in R/RF moves towards small qz, suggesting that the thickness of protein layer becomes thicker during adsorption. More details will be discussed.



Time-resolved X-ray reflection measurements regrame(LSZ) adsorption at the arrivater interface

Keywords: X-ray reflectivity, protein unfolding, SPring-8

## P12.06.18

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### **Resonance shear measurement on liquid crystal** confined between solid surfaces under electric field

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It is known that the properties of liquids confined in the nanometer scale spaces are quite different from those of bulk liquids due to the structuring. We developed a resonance shear measurement<sup>1)</sup>