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The conventional surface x-ray diffraction method [1] allows us to determine atomic arrangements of crystal surfaces and interfaces. While x-ray diffraction intensities distributed within a reciprocal lattice space are usually measured with a finetooth comb using the method, an overall image of the diffraction intensity profile is difficult to get until after such lengthy and time consuming measurement is completed. We proposed x-ray reciprocal-lattice space imaging method (X-ReSI) for straightforward understanding of 1D nanostructures such as NiO nanowires [2]. The X-ReSI is a single-exposure diffraction technique which records the reciprocal-lattice pattern of a fixed crystalline nanostructure using a 2D detector. The fundamental idea behind the method is that the reciprocal lattice of 1D or 2D structures are an array of sheets or rods, respectively. Thus the reciprocal-lattice space can be recorded for a fixed sample with a 2D x-ray detector fixed. The typical exposure time is a few seconds to a few minutes using the 3rd generation x-ray source. We applied the method to structural evaluation of Bi nanolines being 1/8 monolayers in coverage on average. The results of the application reveal that Bi nanolines embeded in Si was found to have a 2 x n superstructure having Bi dimer bonds [3]. On the other hand line structures in samples capped with an amorphous Si layer and having no cap layers still remained with a non-detectable amount of the 2 x n atomic structures. Other applications are structural determination of a $Bi_4Ti_3O_{12}$ thinfilm and in-situ observation of a Au electrode in H_2SO_4.

Keywords: surface x-ray diffraction, baried 1D Bi line, $Bi_4Ti_3O_{12}$ thinfilm

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Precise determination of crystal orientation for surface X-ray diffraction using Kossel line

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We have devoted our efforts toward developing transmission X-ray diffraction (TXD) for surface to realize more time-effective and precise surface structure analysis than the conventional surface X-ray diffraction (Tajiri et al., 2004). The direction of the development is to enlarge a research field by surface X-ray diffraction, e.g. a complex periodic-structure of surface with a large unit-cell which should have a fascinating physical and chemical properties, and not only inert prototypical surfaces but also practical surfaces with a short life-time. In TXD, we observe diffracted X-rays from surface as a pattern by area detector without rocking a sample, as is common with electron diffraction for surface. In this diffraction geometry, it is very reasonable to keep a sample stationary even during determination of crystal orientation from the viewpoint of high-throughput measurement. We report here a stationary determination of crystal orientation using Kossel line (Kossel et al., 1935), which is diffraction by inside source. The experiments were performed at the beamline BL13XU for surface and interface structures in SPring-8. We detected Kossel patterns from a silicon thin substrate by area detector, e.g pixel-array detector (Eikenberry et al., 2003), simultaneously with crystal truncation rod (CTR) scatterings and surface super-structure reflections. By a simultaneous observation of Kossel lines with CTR scatterings and fractional-order reflections, we cat determine crystal orientation necessarily for indexing X-ray diffraction from surface by a single shot.

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Keywords: surface crystallography, surface diffraction, synchrotron X-ray diffraction

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Three-dimensional imaging of interface atoms using crystal-truncation rod scattering

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It is well known that the measurement of X-ray Crystal Truncation Rod (CTR) scattering gives structural information on surface and interface atoms with respect to the substrate crystal. Usually the X-ray intensities observed are compared with the intensities calculated from structural models until the best-fit model is obtained. In this work we study a holographic method to reconstruct three-dimensional images of interface atoms directly from X-ray CTR scattering. The method utilizes the interference effect between the object wave and the reference wave in holography [1]: the object wave corresponds to the X-ray scattering from the known structure and the reference wave to the unknown interface structure to be determined. In the case of hetero-epitaxially grown thin films, the structure of the thin film as well as the substrate crystal is usually known, but the interface structure is a target to be determined. In the present work, we apply the holographic method to study the interface structure of iron-silicide thin films grown on the Si(111) substrate crystal[2]. The calculations show that the interface atoms reconstructed are stable for the structural changes.

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Keywords: interface structure, phase determination methods, crystal truncation rod scattering

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Studies of $FeSi_2$/Si quantum dot nano-structures by X-ray Bragg-surface diffractions (BSD)

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The method of using Bragg surface diffraction (BSD) for structural investigation of thin film/substrate systems has recently been introduced and demonstrated successfully for interfacial strain analysis. With the BSD method, the strain field can be determined by

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: $FeSi_2$, interface, diffraction

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Oxygen-induced D03-sublattice disorder at the Fe_3Al(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_3Al(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^-6 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) ￥AA ￥ 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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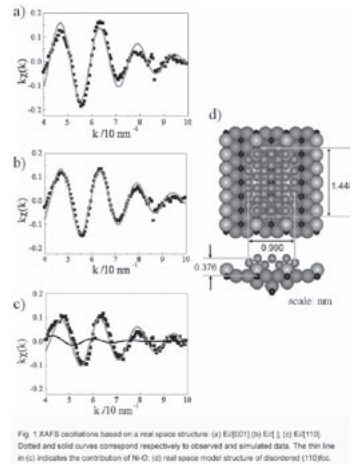
Metal-oxide interaction plays an important role in catalysts, sensors, electric devices, optical materials and so on. Single crystal oxide systems are used as model system and a TiO_2(110) surface is most widely studied. We have investigated Ni on TiO_2 (110) using polarization-dependent total reflection 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

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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.
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