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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