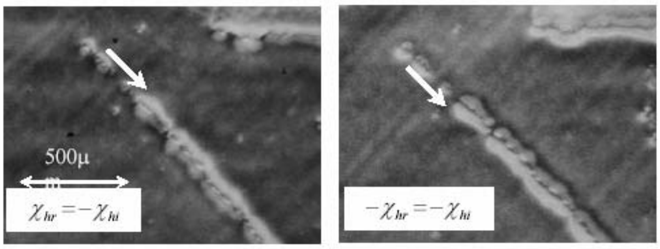
reversed by changing the phase of χ_{hr} and χ_{hi} as shown in the figure below. This clearly shows that such a change of contrast using resonant scattering should be quite useful to analyze characteristics of defects in a crystal.



[1] Negishi R., Yoshizawa M., Zhou S., Matsumoto I., Fukamachi T., Kawamura T., *J. Synchrotron Rad*., 2004, **11**, 266.
Keywords: X-ray topography, resonant scattering, defect contrast

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Characterization of Dislocations in Protein Crystals using Synchrotron White-beam Topography

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To determine three-dimensional structure of protein molecules using X-ray diffraction method and neutron diffraction method, various protein crystals are grown. In particular, large protein crystals (~2 mm) are required for neutron diffraction method since the brilliance of neutron radiation is weak. Moreover, the characterization of crystal defects, especially dislocations, in protein crystals is important for an understanding of their crystallization. Therefore, it is important to establish synchrotron white-beam topography of protein crystals, which is one of the most powerful methods for characterization of dislocations in the large protein crystals. The application of X-ray topography to protein crystals has been carried out by some groups. However, the topographic contrasts observed in protein crystals were poor compared with those in organic crystals of small molecules reported previously. We found that the thickness of protein crystals should be more than 0.4ξ (ξ: the extinction distance) to observe the clear images. Thus, we have succeeded in observing clear topographic contrasts not only in tetragonal hen egg-white (HEW) lysozyme crystals [1] but also orthorhombic HEW lysozyme crystals using large protein crystals (~2 mm). These dislocations structures will be discussed at the conference.

[1] Tachibana M., Koizumi H., Izumi K., Kajiwara K., Kojima K., *J. Synchrotron Rad.*, 2003, **10**, 416.
Keywords: x- ray topography, protein crystals, dislocations

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Quantitative X-ray Diffraction Study of Welded Joints in Heat-resistant Steels

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Welding of cast heat-resistant steels have attracted much attention because of their interesting high-temperature applications in the metallurgical and mining industry. However, welded joints in service at elevated temperatures can yield precipitation of intermediate complex phases such as sigma, chi and carbides. In order to compare the behavior of the material with its microstructural features, a quantitative characterization of the weldments was carried out by means of X-ray diffraction. For this purpose Rietveld analysis were performed on a series of arc-welded joints of heat-resistant steels of the HC (25Cr-3Ni) and HD (30Cr-6Ni) type.

The Rietveld refinements were performed based upon typical measurement and global parameters. The powder diffraction patterns of the weldments resulted in strong preferred orientation effects due to the uniaxial solidification of the weld metal-pool, which was corrected in the Rietveld refinement by using the March-Dollase function. The pseudo-Voigt function was used for the simulation of the peak shapes, while the background was modeled by a 3rd order polynomial in 2θ with refinable coefficients.

A total of five phases were identified and considered in the refinemet process, namely ferrite (Cr,Ni), austenite (Ni,Cr), sigma phase, $Cr_{23}C_6$ and Cr_7C_3.

The main advantage of this processing was the use of the March-Dollase model for correction of the strong texture effects on the diffraction pattern of the weldments, which yield the lower R-values.

Keywords: Rietveld refinemet, welding , heat-resistant steels

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Detection of weak X-ray Waves Scattered by the Crystal Subsurface Inclusions

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In presented theoretical paper a method is proposed appropriate for the non-destructive high-resolution investigations of the various kinds of non-diffracting subsurface nanosize inclusions based on the Grazing-Angle Incidence X-ray Backdiffraction (GIXB) technique [1, 2], which takes place in the conditions of specular vacuum wave suppression phenomenon [3]. Note that in the conditions of the reflected wave suppression mode [3] the specular wave (contrary to other existing X-ray diffraction methods) practically carries the information only about the non-diffracting subsurface inclusions.

Proposed method can be used to register relatively weak X-ray waves scattered by the non-diffracting subsurface inclusions or reflected by the surface regions, which aren't involved in backscatter diffraction process inside the thin crystalline film or the nanostructure.

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Keywords: inclusions in crystal, grazing incidence X-ray diffraction, X-ray backscatter diffraction

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Dislocations and Crystallite Size in Forsterite Produced at 11 GPa and 1400 °C

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Synthetic forsterite is deformed at 11 GPa, 1400 °C in a multianvil high pressure apparatus at the Bayerisches Geoinstitut (Universität Bayreuth, Germany). X-ray diffraction patterns are measured by a special high resolution double crystal diffractometer with negligible instrumental effects. The monochromatised $K\alpha_1$ beam has a footprint on the specimen of 0.1x1 mm^2, enableing microbeam analysis. This condition provides diffraction patterns of the small specimens of the size of 0.2x2 mm^2. High resolution enables to carry out line profile analysis on the reflections well separated from those of platinum and corrundum unavoidable due to the small compact specimen structure. The dislocation densities are found to decrease with holding time at 1400 °C from about between 16×10^{14} m^{-2} to 0.04×10^{14} m^{-2}. Good correspondence of the dislocation structure determined by X-ray line profile analysis and TEM observations has been established [1].

[1] Couvy H., Frost D., Heidelbach F., Nyilas K., Ungár T., Mackwell S., Cordier P., *European Journal of Mineralogy*, 2004, **16 (6)**, 877-889.

Keywords: dislocation structure, microbeam analysis, high resolution X-ray diffraction

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X-ray Synchrotron Studies of AlGaAs Based Laser Structures

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Modern semiconductor lasers include a complicated layered structures with quantum wells and insulated buried layers introduced by selective implantation with He or H ions. The strain and defects induced by implantation may disturb the action of the laser. In present studies the most important methods of characterization were white beam Bragg case section topography and recording of rocking curves with a small 50×50 μm^2 probe beam.

The investigations were performed in a special multilayers containing two relatively thick layers of AlGaAs separated by a thin layer with smaller Al concentration, covered by 0.3 μm GaAs cup. The structures were studied before and after implantation with 150 keV He ions at room temperature and 180º C. It was possible to reproduce the character of experimental rocking curves in numerically simulated using the Takagi-Taupin theory. In the computations we included the change of chemical composition and a strain profile being a sum of strain connected with epitaxial layers and the point defect distribution obtained with TRIM95. The necessary modification of the point defects distribution was flattening of the top part.

The section topographs revealed stripes due to successive epitaxial layers and the strain modulation fringes due to the buried layer. In case of selective implantation the topographs revealed some contrasts due to strains at the edges of the implanted areas.

Keywords: defects, semiconductor structures, diffraction

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Strain Profiles in the Insulated Buried Layers Obtained by He Implantation in AlGaAs

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The insulated buried layers formed by 150 keV He ions to $Al_xGa_{1-x}As$ with various concentration of Al were studied with synchrotron diffraction methods. Some samples were studied with HRTEM. The implantations were performed at RT, 80 and 120º C. The doses varied from 2×10^{16} to 6×10^{16} cm^{-2}. The measurements included taking local rocking curves using small 50×50 μm^2 probe beam. The rocking curves exhibited characteristic interference maxima and enabled the analysis of the strain profiles by fitting the theoretical rocking curves obtained by numerical integration of the Takagi-Taupin equations. The white beam synchrotron back reflection topography revealed a sequence of strain modulation fringes similar to the main interference maxima in the rocking curves. The evaluated profiles exhibited the deformed region close to the surface indicating that the deformation is mainly caused by the point defects produced by incident ions and the recoils. The other feature increasing with the temperature of implantation was the flattening of top part of the strain maximum corresponding to the insulating buried layer. This flattening was more distinct for lower concentration of Al. The HRTEM patterns revealed characteristic small gaseous inclusions appeared in the most deformed region in the samples implanted with the highest applied doses.

Keywords: strain, ion implantation, diffraction

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Huang Diffuse Scattering by Mesoscopic Interstitial Defects in BCC Metals

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Microstructural evolution of materials in the extreme environment of a fusion or an advanced fission power plant is driven by migration of defects produced by irradiation. If the energy of collision cascades is low, only point defects (vacancies and single interstitial atoms) are generated. Agglomerating point defects form dislocation loops and voids. Huang diffuse scattering (HDS) is used for the determination of structure of single interstitial defects generated by irradiation.

We show that in addition to single interstitial atom defects, mesoscopic defect clusters containing two or more interstitial atoms give a strong contribution to the observed HDS patterns. The occurrence of clusters of interstitial atoms in e-irradiated bcc iron was proved in a recent study of resistivity recovery curves. The effect of interstitial atom clusters on HDS has not yet been investigated. The size of these clusters is comparable with the lattice constant making the infinitesimal dislocation loop approximation underlying the existing treatment of HDS not applicable. We show that the fact that the core of a mesoscopic interstitial cluster is fully three-dimensional has a strong effect on the long-range elastic strain field, and this masks the symmetry-related features of HDS associated with single interstitial atom defects. The new findings may help resolving the conflict between predictions of density functional calculations and the existing interpretation of experimental observations of HDS in bcc metals of the VIth group of the periodic table.

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Keywords: diffuse scattering, defect structures, defect clusters

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XRD Peak Profiles in the Case of the Lognormal Crystallite Size Distribution

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Since the lognormal distribution of a crystallite size in a powder simple is the most realizable one in practice, determination of the size distribution parameters (the median and logarithmic standard deviation) from X-ray diffraction peak profile characteristics (FWHM or integral width and shape factor) is an important problem of structure analysis.

Langford *et al*. [1] have shown in principle that the size distribution can be determined directly by a profile fitting method. However, their evaluation restricted to a small variance of the distribution.

In this paper, effect of the lognormal distribution parameters on the peak profile is examined without any assumption of the parameter rage. For that the diffraction peak intensity profiles from lognormally distributed spherical crystallites is simulated and analyzed thoroughly.

Unique correlation between the distribution parameters and the XRD peak characteristics was found to exist within a wide range of the parameter values.

[1] Langford J.I., Louer D., Scardi P., *J. Appl. Cryst.*, 2000, **33**, 964.

Keywords: powder, crystallite size distribution, XRD

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Evolution of Nanostructure States of Cu-powders Prepared by Ball Milling

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