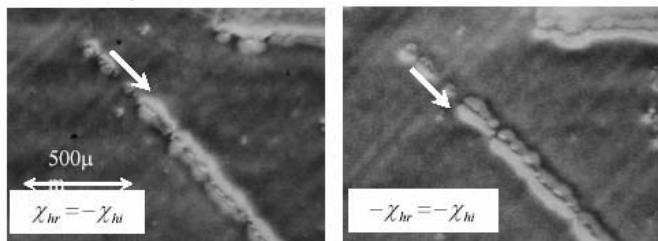


reversed by changing the phase of χ_{hr} and χ_{hi} as shown in the figure below. This clearly shows that such a change of contrast using resonant scattering should be quite useful to analyze characteristics of defects in a crystal.



[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

P.17.03.3

Acta Cryst. (2005). A61, C448

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

Kenichi Kojima^a, Haruhiko Koizumi^a, Miki Shimizu^a, Masaru Tachibana^a, Kentaro Kajiwara^b, Hiroshi Sugiyama^c, ^aGraduate School of Integrated Science, Yokohama City University. ^bSpring-8/JASRI. ^cPF/KEK. E-mail: kojima@yokohama-cu.ac.jp

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 dislocation 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

P.17.04.1

Acta Cryst. (2005). A61, C448

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

Jorge L. Garin, Rodolfo L. Mannheim, *Department of Metallurgical Engineering, University of Santiago de Chile, Santiago, Chile.* E-mail: jgarin@lauca.usach.cl

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 refinement 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 refinement, welding, heat-resistant steels

P.17.04.2

Acta Cryst. (2005). A61, C448

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

Hakob P. Bezirganyan^a, Hayk H. Bezirganyan (Jr.)^b, Siranush E. Bezirganyan^c, Petros H. Bezirganyan (Jr.)^d, ^aDepartment of Solid State Physics, Faculty of Physics, Yerevan State University, Yerevan, Armenia. ^bFaculty of Computer Science and Applied Mathematics, Yerevan State University, Yerevan, Armenia. ^cDepartment of Medical & Biological Physics, Yerevan State Medical University after Mkhitar Heratsi, Yerevan, Armenia. ^dDepartment of Computer Science, State Engineering University of Armenia, Yerevan, Armenia. E-mail: hakob_bezirganyan@yahoo.co.uk

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.

[1] Bezirganyan H.P., Bezirganyan P.H., *Phys. Stat. Sol. (a)*, 1988, **105**, 345.

[2] Bezirganyan H.P., *Phys. Stat. Sol. (a)*, 1988, **109**, 101. [3] Bezirganyan H.P., Bezirganyan H.H. (Jr.), Bezirganyan S.E., Bezirganyan P.H. (Jr.), *Opt. Comm.*, 2004, **238/1-3**, 13.

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

P.17.04.3

Acta Cryst. (2005). A61, C448-C449

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

Krisztián Nyilas¹, Hélène Couvy^{2,3}, Patrick Cordier^{2,3}, Tamás Ungár¹, ¹Department of General Physics, Eötvös University Budapest, H-1518, POB. 32, Budapest, Hungary. ²Bayerisches Geoinstitut, Universität Bayreuth, Germany. ³Laboratoire de Structure et Propriétés de l'Etat Solide, ESA CNRS 8008, Université des Sciences et Technologies de Lille, Villeneuve d'Ascq, France. E-mail: nyilas@metal.elte.hu

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 $0.1 \times 1 \text{ mm}^2$, enabling microbeam analysis. This condition provides diffraction patterns of the small specimens of the size of $0.2 \times 2 \text{ mm}^2$. High resolution enables to carry out line profile analysis on the reflections well separated from those of platinum and corundum unavoidable due to the small compact specimen structure. The dislocation densities are found to decrease with holding time at 1400 °C from about between $16 \times 10^{14} \text{ m}^{-2}$ to $0.04 \times 10^{14} \text{ m}^{-2}$. Good correspondence of the dislocation structure determined by X-ray line