FA5-MS38-P01

High-Brilliance Home-Lab X-Ray Sources: Status and Future. Jörg Wiesmann, Carsten Michaelsen, Jürgen Graf, Bernd Hasse, Incoatec GmbH, Max-Planck-Strasse 2,21502 Geesthacht, Germany E-mail: wiesmann@incoatec.de

Modern microfocus X-ray sources define the state-of-the-art for a number of applications such as protein crystallography and small-angle scattering in the home lab. These sources have small source sizes of 100 μ m or smaller. They are usually combined with multilayer mirrors as beam-shaping devices that image the source spot onto the sample position, magnified to a suitable size, and deliver a parallel or focused monochromatic beam.

Microfocusing rotating anode systems deliver flux densities in the range of 10^{11} photons/(s mm²) at power loads of up to 20 kW/mm² when combined with synthetic multilayer mirrors [1]. However, these sources are expensive, and need regular and sometimes time-consuming maintenance.

Low power microfocus sealed tube sources such as the Incoatec Microfocus Source "I μ S" represent an interesting low-maintenance alternative to rotating anode generators. Power loads of several kW/mm² in anode spot sizes of \leq 50 μ m deliver a small and highly brilliant beam [2]. The I μ S delivers a flux density of up to 10¹⁰ photons/(s mm²) in a focused beam (FWHM = 0.11 mm, 7.6 mrad) suitable for most protein crystals.

Emerging microfocus X-ray sources based on liquid-metal-jet technologies show even higher power loads up to 500 kW/mm^2 , an order of magnitude higher than possible with solid target sources, and intensities up to 10^{12} photons/(s mm²) together with a relatively low power consumption and reduced maintenance [3].

We will present selected results from several microfocus source systems to demonstrate their potential for crystallography and small-angle scattering.

[1] Durst R., Storm A., *Technical Note SCD 4 from Bruker AXS*, 2007, DOC-T86-EXS004. [2] Wiesmann J., Graf J., Hoffmann C., Hembd A., Michaelsen C., Yang N., Cordes H., He B., Preckwinkel U., Erlacher K., *Part. Part. Syst. Charact.* 2009, 26 (3), 112. [3] Otendal M., Tuohimaa T., Vogt U., Hertz H.M., *Rev. Sci. Instr.*, 2008, 79, 016102.

Keywords: X-ray microfocus source, X-ray reflective multilayers, X-ray diffractometry

FA5-MS38-P02

Peculiarities of x-ray multiwave diffraction in paratellurite crystals (TeO2). <u>A.E.Blagov</u>^a, M.V.Kovalchuk^{a,b}, V.G.Kon^b, P.A.Prosekov^a, Yu.V.Pisarevskij^a, ^a *A.V.Shubnikov Institute of Crystallography Russian Academy of Sciences*,

Moscow, Russia, ^bRussian Research Centre «Kurchatov Institute»

The interference effects under multiwave X-ray diffraction [1] have been studied in paratellurite single-crystal (TeO2). The calculation of three-beam diffraction schemes was carried out for complanar or near-complanar geometry. Three combination of x-ray reflections (220, 371), (220, 464) and (110, 557) were obtained and used for the multibeam

diffraction research. All three cases have been experimentally realized by applying a scheme of high-resolution double crystal X-ray diffraction using a laboratory source (Mo K1). The most interesting results were obtained for the case of (220, 371) reflections. Unlike (220, 464) and (110, 557) cases, a strong effect of virtual scattering [2] was observed for (220, 371) reflections. One characteristic feature of this effect is that the angular dependence of the first (strong) reflection intensity and its shape barely change in the three-beam interaction area. whereas very strong changes are observed for the second (weak) reflection not only in the three-beam range but also far beyond it. Such strong changes are related to the variation in parameter of the two-beam diffraction due to virtual scattering. In (220, 464) and (110, 557) three-beam cases this effect was practically absent and purely amplitude scattering (ordinary multiwave interaction) [2,3] took place. The results of experimental observation of investigated effects for all three cases of (220, 371), (220, 464), (110, 557) three-beam diffraction would be presented. The results of computer modelling in comparison with experimental data for (220, 371) three-beam diffraction would be presented also.

The work was supported by RFFI (grants 09-02-12164-ofi_m, 09-02-12239-ofi_m) and RF President (grant MK-156.2010.2).

[1] S.L. Chang, Berlin, Springer, 1984. [2]. V. G. Kohn, Sov. Phys. Crystallogr., 1988, 33, 333. [3] A. E. Blagov, M. V. Kovalchuk, V. G. Kohn, Yu. V. Pisarevskii, and P. A. Prosekov, Crystallography Reports, 2010, 55, N 1, 10.

Keywords: multiwave X-ray diffraction, double crystal diffractometry, X-ray diffraction theory

FA5-MS38-P03

Probing gels as a media for the growth of co-crystals. <u>Duane Choquesillo-Lazarte</u>^a, Juan Manuel García Ruiz^a, ^aLaboratorio de Estudios Cristalograficos, IACT-CSIC, Spain

E-mail: duanec@ugr.es

The interest in co-crystals has increased in the last years within the pharmaceutical industry and also the solid-state community due to the possibility of obtaining solid materials with new properties [1]. Co-crystal crystallization strategies, supported by solvent- and solid-based techniques, have also received attention in the search and development of robust methodologies for the screening of co-crystals. This work explores the use of gels in a solvent-based approach to obtain co-crystals. The use of gels as a media permitting diffusive mass transport has been reported for the crystallization of small molecules [2] and proteins [3]. A series of co-crystals obtained using model molecules and selected co-crystals formers and grown in water- and/or organic solventcompatible gels will be presented.

[1] Blagden, N., Berry, D.J., Parkin, A., Javed, H., Ibrahim, A., Gavan, P.T., De Matos, L.L., Seaton, C.C., *New J. Chem*, 2008, 32, 1659. [2] Henisch, H.K., *Crystal Growth in Gels and Liesegang Rings*, Cambridge University Press, Cambridge (1988) [3] García-Ruiz, J.M., *J. Crystal Growth*, 2001, 232, 165.

Keywords: gels, crystallization, co-crystals