

## Diffraction Physics I Neutron & X-Ray Optics

**MS15.01.01 HIGH-RESOLUTION HIGH-LUMINOSITY TECHNIQUES FOR NEUTRON SCATTERING BASED ON BENT CRYSTAL MONOCHROMATORS.** Mihai Popovici, William B. Yelon and Ronald R. Berliner, Missouri University Research Reactor

Neutron scattering instruments measure scattering laws  $S(\mathbf{Q})$  or  $S(\mathbf{Q}, h\omega)$ , the variables being the wave-vector transfer  $\mathbf{Q}=\mathbf{k}_i-\mathbf{k}_f$  and the energy transfer  $h\omega=E_i-E_f=h^2(k_i^2-k_f^2)/(2m)$ . Conventional instruments try hard to precisely define both the incident and scattered wavevectors  $\mathbf{k}_i$  and  $\mathbf{k}_f$  with the aid of Soller collimators. This leads to large losses and to the neutron scattering being intensity limited even at the highest flux sources available.

Unconventional instruments with focusing monochromators have been developed recently. Their basic idea is to precisely define not  $\mathbf{k}_i$  and  $\mathbf{k}_f$  separately, but the combinations  $\mathbf{Q}$  and  $h\omega$  only. This is done by controlling the correlations between  $\mathbf{k}_i$ ,  $\mathbf{k}_f$  and the sample coordinate  $\mathbf{r}$  with bent crystal monochromators. The theory, expressed in matrix language, is based on considering the  $(\mathbf{k}_i, \mathbf{r}, \mathbf{k}_f)$  space and then making the transformation to the  $\mathbf{Q}$  or  $(\mathbf{Q}, h\omega)$  space. The potential of focusing techniques is far from being fully explored and some necessary tools have yet to be developed.

The special features of focusing instruments are:

- resolution is set by the sharpness of the correlations, thus by the crystal reflectivity widths and the sample size (thickness, with plate samples);
- beams are fully open (no Soller collimators), leading to high luminosity;
- gains over conventional instruments in both intensity and resolution are possible (intensity may not be sacrificed for resolution and vice-versa);
- high resolution is obtained with bent perfect crystals of narrow reflectivity;
- resolution can be traded for intensity by using mosaic crystals;
- focusing in scattering with open beams can be combined with real space focusing of neutrons onto small samples (Liouville theorem still obeyed);
- focusing monochromators make a perfect match with position sensitive detectors;
- cold sources are not mandatory for high resolution work, thermal sources may be OK.

**MS15.01.02 POLYCAPILLARY OPTICS FOR NEUTRONS AND X RAYS.** D.F.R. Mildner, H. H. Chen-Mayer, National Institute of Standards and Technology, Gaithersburg, MD 20899, and R.G. Downing, V.A. Sharov and Q.F. Xiao, X-Ray Optical Systems, Inc, Albany NY 12205

The principle of multiple mirror reflection from smooth surfaces at small grazing angles makes it possible to transport slow neutrons and x rays with high efficiency using narrow tubes. Such a mechanism provides the opportunity to bend and focus the radiation on a scale suitable for laboratory needs. Recent developments in glass polycapillary fibers with thousands of channels having sizes of a few microns have enabled the radiation to be focused to submillimeter spot sizes for neutrons.

A neutron focusing lens can enable an increased spatial resolution and an improvement in the detection limits for individual elements for absorption techniques in analytical and materials research (such as neutron depth profiling and prompt gamma activation analysis). The following parameters have been considered in the design of the focusing lens: the depth of focus,

determined by the beam width as a function of distance from the lens, the optimum focal length, obtained by maximizing the current density at the focus for a given size of the focal spot, and a shift in the neutron energy spectrum of the transmitted beam relative to the incident beam, since curved channels preferentially transmit longer wavelength neutrons.

We have constructed a lens using polycapillary glass fibers for focusing a large area neutron beam (50 x 45 mm<sup>2</sup> corresponding to the exit dimensions of a <sup>58</sup>Ni guide) to spot of width ~ 0.5 mm at a focal distance of 52 mm with a current density gain of 80. A series of images of the transmitted beam taken at progressively greater distances from the lens exit indicates the convergence of the output of the fibers and their subsequent divergence beyond the focal point. The shape of the profile at the focus has a Gaussian distribution with a full-width at half-maximum of 0.54 mm.

Prompt gamma measurements using the focused beam have been performed to demonstrate the enhanced sensitivity and lateral resolution. The gain in  $\gamma$ -ray count rate is about 60, and though the background from unfocused neutrons is increased, the sensitivity of detection is increased by a factor of 20. Recent developments in x-ray focusing will also be discussed.

**MS15.01.03 SECONDARY EXTINCTION OF X-RAY AND NEUTRON DIFFRACTION IN MOSAIC CRYSTALS\*.** Hua-Chen Hu, China Institute of Atomic Energy, P. O. Box 275(18), Beijing 102413, People's Republic of China

Universal expressions by using three dimensionless parameters for the secondary extinction factors in X-ray and neutron crystallography are developed based on the exact solutions of the power transfer equations. These methods can be applied to reflections of all possible values of extinction factor, reflection symmetry and the absorption to scattering cross-section ratio of the crystal. The representation by three parameters gives a clear and definite physical meaning to the concept of extinction. The theory has been extended to treat the extinction of a spherical crystal. As a demonstration of the feasibility of using these expressions, the diffraction data on LiF and MgO plane mosaic crystals measured by Lawrence [(1972) Acta Cryst. A28, 400-404, and (1973) Acta Cryst. A29, 208-210.] are reanalyzed by this method. All the reflections including the strongest ones ( $Y_0$  down to 0.026) are reanalyzed simultaneously with single-valued particle size and mosaic spread as fitting parameters and allowing for primary extinction if necessary. The results (R factor = 0.014 and 0.053 for LiF and MgO, respectively) are unprecedentedly good. Furthermore, in disagreement with Lawrence, the extinction of LiF is found to be of secondary type, and in the case of MgO both primary and secondary extinction should be considered. The analysis shows that Darwin's transfer equations are valid in a range much broader than previous anticipated.

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