13. NEUTRON DIFFRACTION

13.X-1  THE PRODUCTION OF NEUTRONS BY SPALLATION SOURCES. By C. G. Minderer, Materials Physics Division, AERE, Harwell, Oxford OX11 0RA, UK.

At the present time we are in a time of strong expansion in neutron sources using accelerator based pulsed proton spallation. The progress over the last few years and the probable growth over the next few years will be reviewed. The sources with very short proton pulses offer performance (counts per given resolution) essentially independent of neutron energy over the epithermal range. The present fruits of this will be reviewed for diffraction and inelastic scattering. Speculations will be given on how these may be extended over the next few years. The longer proton pulse sources offer very high peak thermal fluxes and are well suited to the production of cold neutrons, which have a long intrinsic moderation time. The performance of experiments suited to these sources will be compared with these on shorter pulsed sources and on reactors.

13.X-2  HIGH-RESOLUTION POWDER DIFFRACTION AT PULSED NEUTRON SOURCES. By James D. Jorgensen, Argonne National Laboratory, Argonne, IL 60439, USA.

The recent development of accelerator-based pulsed neutron sources has made possible the design and operation of time-of-flight powder diffractometers which achieve high resolution and count rates. Since no chopper is used, the sample can view a large source area. Thus, long source-to-sample flight paths can be used to obtain high resolution. The pulse repetition rate is typically low enough to avoid frame overlap. Count rates are maximized by combining detectors into time-focussed groups. In the most recent diffractometers, time focussing is accomplished by in-line micro-computers rather than geometrical methods and can be done at any scattering angle. Rietveld structural refinement of data from these instruments requires a precise description of the incident neutron flux versus wavelength and of the peak shape. The peaks are non-Gaussian and asymmetric, with the width being roughly proportional to wavelength. However, suitable analytical functions which adequately model the peak shape and its wavelength dependence have been developed and Rietveld refinement of pulsed-source, time-of-flight data is now routinely done. When used at a pulsed neutron source, the time-of-flight method allows a large range of reciprocal space to be viewed simultaneously. The resolution at a given scattering angle is nominally constant. Since complete data can be obtained at a single scattering angle, the time-of-flight method also offers advantages for diffraction in restricted environments.

This work has been supported by the U.S. Department of Energy, Division of Materials Research under contracts DE-AC02-76ER01198 and W-31-109-ENG-39.

13.X-3  THE APPLICATION OF SPALLATION NEUTRON SOURCES FOR INELASTIC SCATTERING. By B. Alefeld, Kernforschungsanlage Jülich, Germany.

The most important characteristic feature of a Spallation Neutron Source is the possibility of time dependent neutron production. The time dependent structure of the neutron flux leads to a direct advantage for the time-of-flight methods. This has been demonstrated impressively at the existing Spallation sources at Argonne (USA), Los Alamos (USA) and KEK (Japan) where results have been obtained, which could not or only hardly be obtained at the existing High Flux Reactors where the time averaged flux is much higher. It will be shown, that also other important spectroscopic techniques which are successfully used on steady state sources like Triple Axis Spectroscopy, Back-Scattering, Small Angle Scattering and Spin Echo-Spectroscopy gain by the time dependent neutron flux of a Spallation Neutron Source (compared to a steady state source with the same average flux). The time dependent neutron flux of a Spallation Source probably will cause a revival of promising spectroscopic methods like the correlation spectroscopy and certainly is a strong stimulation for developing new experimental methods, leading to a better neutron economy for scattering experiments than is possible on continuous neutron sources. A new type of a time of flight instrument is described, in which phase space transformation is combined with time focusing leading at least theoretically to pulse intensities which are much higher than at existing time of flight instruments.

13.1-1  A NEW LINEAR POSITION-SENSITIVE SCINTILLATION DETECTOR FOR NEUTRONS. By W. Schäfer, E. Jansen and G. Will, Mineralogisches Institut, Universität Jülich, Universität Bonn, Bonn, W.-Germany.

The technique of the linear scintillation position-sensitive detector (PSD) is based on the principle of the gamma-ray Anger camera modified by new electronic processing and stabilisation methods to the requirements for application in neutron powder diffractometry [Schelten, J., Kurz, R., Naday, I. and Schäfer, W., Nucl. Instrum. Methods (1983) 205, 319; Naday, I. and Schäfer, W., (1983) Proc. of the Workshop on Position-Sensitive-Detection of Thermal Neutrons, Grenoble, 1982 (Academic Press, London) in the press]. The scintillator material is Li-enriched glass of 1 mm thickness with a detection probability for 1.3 A neutrons of about 75%. One PSD unit has a sensitive length of 882 mm using 24 photomultiplier tubes of 1 1/8" diameter each. The spatial resolution of the PSD expressed by the width of the response function is 2.5 mm (FWHM). The integral linearity is better + 0.1 mm. The pulses of one PSD unit are registered in T024 channels. The channel to channel variation along the PSD is + 1.5% according to a primary calibration by an homogeneous illumination with neutrons. The gamma-sensitivity of the Li-glass scintillator is minimized by electronic pulse height discrimination to lower 10^-4.

Two identical PSD units (one is shown in the figure) are installed on the powder diffractometer KATINNA in the research reactor D100 in the KFA Jülich. It is possible, to vary the distance PSD-sample continuously between 115 and 190 cm corresponding to 20-ranges of about 30^0 and 20^0 resp. for each unit, thus varying the angular resolution of the PSD from 0.12^0 to 0.07^0 resp. The angular separation of the two units is also
variable; usually they are mounted with a dead zone in between of about 20° in 28. The whole PSD arrangement can be rotated with an accuracy of 0.01° in order to measure the dead zone in a second step.

The specific features of the powder diffractometer equipped with the scintillation PSD are: 1. High efficiency also in the region of shorter wavelengths λ<2λc<1.5 A, thus (a) using wavelengths in the maximum of the intensity distribution of the thermal reactor spectrum, (b) suffering low λ/2-contamination due to the rapid decrease of the reactor spectrum to higher energies, (c) having sufficient coverage in reciprocal space for structure analysis also for confined scattering geometry. 2. With λ/dλ-values for the PSD of 1% to 0.1% (10^4<2θ<100°) the detector is, in general, not the limiting element in the angular resolution of the diffractometer. 3. High data point density in the diffractograms (e.g. 40 data points per degree 28) for a successful application of peak profile analysis methods (Mill, G., Jansen, E. and Schäfer, W., (1982) AIP Conf. Proc. No 89, Neutron Scattering-1981, 205).

13.1-3 A HIGHLY EFFICIENT DOUBLE-CRYSTAL MONOCHROMATOR FOR THERMAL NEUTRONS. By F. Mikula, J. Kulda and B. Chalupa, Nuclear Physics Institute, 250 68 Rež near Prague, Czechoslovakia.

The use of elastically deformed (usually bent) perfect crystals as neutron monochromators has been restricted owing to a rather low "effectiveness" δ0 in comparison with that of conventional mosaic monochromators. This drawback may be overcome through the employment of a stack bent crystal slices (Rekveld, Nucl. Instrum. Meth. (1983) 216, 521). Another way of increasing δ0 is the use of a bent perfect crystal plate in a strongly asymmetric diffraction geometry. The associated effect of the reflected-beam widening is compensated for by the second bent crystal in the parallel (1,-1) setting in the opposite geometry (Mikula, Kulda, Vrána and Chalupa, J. Appl. Cryst. (1984), in press). Then the double diffracted beam has the same dimensions as the incident polychromatic one. The integrated reflectivity ρ0 of such a double crystal (DC) system may be written as

$$\rho_0 = \delta_0 \cdot \rho \cdot R \cdot \alpha(\mu)$$

where δ0 is the total change in Bragg angle for the incident beam on the path through the crystal, R is the peak reflectivity (Kulda, Acta Cryst. (1984), in press) for a given radius R and α(μ) is the attenuation factor depending on the attenuation parameter μ. In case of fully asymmetric geometry when the incident beam enters the crystal through its end face and passes through it along its longest edge, we get δ0 = L/R, R(μ) = (1 - exp(-μl)), α(μ) = exp(μL), where L is the length of the crystals. The extremum of the function ρ0 yields an optimum length L0f in the form L0f = (dθ0/θ0) log(1 + 20(θ0/2θc)). The following figure displays the dependencies of ρ0, L0f and Rf on the wavelength A for Si crystal and fixed dθ0.

The advantages of this DC monochromator based on elastically bent perfect Si crystals may be found in its simplicity, easy control of the effective mosaicity and the integrated reflectivity, low amount of a higher order contamination, low background inherent in all DC monochromators and filtering properties (Fried, Nucl. Instrum. Meth. (1983) 216, 521) when preferably rejecting fast neutrons from the incident polychromatic beam. The drawback of this DC monochromator is in the width of the output monochromatic beam (~50 mrad) given by the thickness of the crystals. This restriction may be solved by replacing each of the crystals with a packet of several crystal slabs.

The results of preliminary experiments have fully confirmed the theoretical predictions.

Photograph of one scintillation PSD unit.


A full-circle Eulerian cradle has been constructed for neutron diffraction measurements on single crystals in the temperature range from liquid helium to room temperature. The whole mechanics of the oradle including the stepping motors of the phi- and chi-rotation is mounted inside the low temperature chamber of a helium cryostat. The positioning accuracy is 0.01° in chi and 0.02° in phi. For constant 4 F measurements the liquid helium level is maintained around 2 cm below the crystal thus avoiding the neutron beam passing through the liquid helium.

The inner diameter of the chi-circle is 175 mm. Goniometer heads up to 52 mm in height M standard threads can be mounted. The two circles and the worm wheels are made of red brass, produced by centrifugal casting process thus minimizing distortion and anisotropical thermal contraction. The worm shafts are made of beryllium copper bronze and the teeth of the gears are covered with gliding varnish in order to reduce friction. The 2 stepping motors are modified for use in liquid helium. The electrical wires are coated with low temperature resistant and flexible insulation. The main applications of this low temperature oradle are crystal and magnetic structure investigations with neutrons. The dimensions of the device allow in future the installation of a high pressure cell on the goniometer head position. By modification of the surrounding cryostat this Eulerian cradle may also be used for X-ray structure analysis.