H1. SUPER-6T2, A NEW POSITION SENSITIVE DETECTOR POLARIZED NEUTRONDIFFRACTOMETER

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Polarised neutron diffraction (PND) is an important technique to investigate interatomic or intermolecular magnetic interactions. PND takes full advantage of the neutron magnetic moment and gives a direct access to the spin density distribution in the unit cell. In contrast to electron density, usually determined from high precision X-ray diffraction techniques, the spin density distribution is directly related to the unpaired electrons. Thus, by comparing spin and electron densities, one can get insights into magnetic interactions. The PND has been extensively used at LLB using the 5C1 diffractometer. Recently it has been successively applied to the studies of anomalous spin densities in ruthenates [1], of the origin of the field-induced ferro-metalic state in bilayer manganites [2], of staggered field effects in the one-dimensional antiferromagnet [3], of photoinduced molecular switching compound [4].

PND is also traditionally of particular interest for the community of chemists working in the field of molecular magnetism. Thus spin density studies in molecule-based magnetic compounds have permitted to obtain a very important information about the magnetic interactions in : ferromagnetically coupled copper(II) dimers [5]; ferromagnetic superexchange through the non-magnetic Ti(IV) ion in a Ti(IV)-(semiquinone)2 biradical [6] and the nature of the interaction in a Mn(II)-Ni(II) ferromagnetic chain compound [7]. Running a PND experiment is quite time consuming thus an improvement of PND diffractometers, which would boost the data acquisition rate, and as a consequence the precision of the information on spin densities is highly desirable.

Hence a new polarized neutron diffractometer has been commissioned at the ORPHEE reactor in Saclay. The instrument is installed on the thermal beam tube 6T2 at the ORPHEE reactor. Vertically focusing pyrolytic graphite is used to select the neutron of wavelength λ= 1.4 Å. The incident monochromatic beam is polarized with supermirror bender installed inside the monochromator protection. The bender has been designed and constructed in PNPI, Gatchina. It consists of 19 channels, each of 0.85 mm width, 50 mm height and 780 mm length. The supermirrors are deposited on 0.3 mm thickness glass and mounted with spacers of 0.85 mm thickness. An additional nonpolarizing supermirror focusing condensor can be inserted in the RF adiabatic flipper, when small samples are used. An adiabatic radiofrequency flipper [8] is installed between the polarizer and superconducting magnet of 7.5 Tesla, see Fig.1. The magnet is equipped by: ³He insert, CuBe pressure cell, very high pressure (sapphire) cell, kappa-geometry and photo-excitation inserts.

To reduce the scattering from the sample environment a radial collimator is installed in the detector protection (Eurocollimators Ltd) and covers 30° in vertical and horizontal directions. We found that the radial collimator reduces the scattering from the sample environment by a factor 10-20, which is of great importance for the performance of the diffractometer, working essentially in extreme sample conditions.
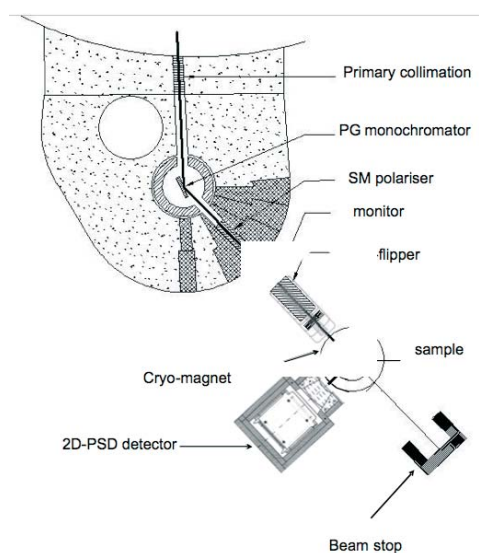

Figure 1. Schematic illustration of the Super-6T2 diffractometer.

The polarization of the incident beam was tested using CoFe single crystal and was found to be P_0=97% (Flipping Ratio ~70). Measurements on bench mark single crystals of CoFe and Ni using single counter, have shown the intensity gain of a factor of 15 compared to the intensity of existing polarized neutron diffractometer 5C1 at LLB. This gain factor will be increased even more with the use of the PSD. In this setup, the diffracted beam is collected by position sensitive multiwire gas detector BIDIM26 developed in ILL [9], fabricated by INEL and bought with the financial support of "Rennes Metropole". It is an individual readout square Multi-Wire Proportional Chamber (MWPC) with a single gas volume. The number of readout channels is (128X * 128Y), with resolution 2*2 mm. The vertical and horizontal acceptance angles of the PSD detector are 25°x25°, (0.19 steradian).

Spinning of sample and collecting of 2D images at only four consecutive detector positions will provide both integrated intensities and flipping ratios up to sin (J/l) ~ 0.6 Å-1 in the horizontal plane and sin (J/l) ~ 0.2 Å-1 in the vertical one. Then for the frames having low statistical accuracy flipping ratios will be re-measured with a longer exposure time to reach the required accuracy. Once the data collection is finished, the vertical axis of the crystal can be driven into the horizontal plane by using kappa-goniometer inserted in the magnet and the missing reflection intensities along the originally vertical crystal axis can be measured.

Data acquisition is realized by means of a EuroPsd microprocessor module designed at the LLB. The module assures connection between the driving computer and the ILL PSD interface via the IEEE 488 bus. It is able to sustain very high acquisition rates (up to 5 Mhz) and to run in different modes, like polarized neutrons, Time Of Flight (TOF) and time resolved modes. The module is equipped by an onboard (16 bit) memory adapted for detector sizes up to 512x512 channels. This makes the acquisition being totally independent from the performance and capacities of the driving computer.

Data are collected using a VISUAL BASIC (VB) software developed in LLB. We chose an industrial standard XML (Extended Markup Language) to store the data collected from the PSD. This standard describes in an easy and intuitive way how the information is stored. It has an advantage as well that it comes with ready made parsers and standard XML editors. The XML file created by the LLB acquisition software contains compressed data collected from the PSD and all current parameters of the diffractometer; date, time, angles, monitor, temperature etc. Visualization program, see Fig. 2, written in JAVA gives quasi-instantaneous visualization and access to any selected frame due to the XML standard, providing tabulation files. The same program assures: reading of frame content, binning and summation of frames and creation of dynamic mask of strongest pixels. Program for indexing, integration and flipping ratio calculations is written in Fortran 90 and MATFOR 4.

For the crystals having small lattice parameters the gain from using the PSD will be very small. In this case we consider a possibility to use several single crystal of different orientation simultaneously. In particular if crystals are mounted at different height, the Friedel pairs can be used to define the zero offsets in the horizontal plane and to separate reflections belonging to different crystals.

Quite large detector aperture (0.19 steradian) allows to measure polarized neutron diffraction from powder samples with a high efficiency. We note that its acceptance angle is nearly four times larger that that of the existing powder diffractometers G4.1 and G6.1 at LLB.
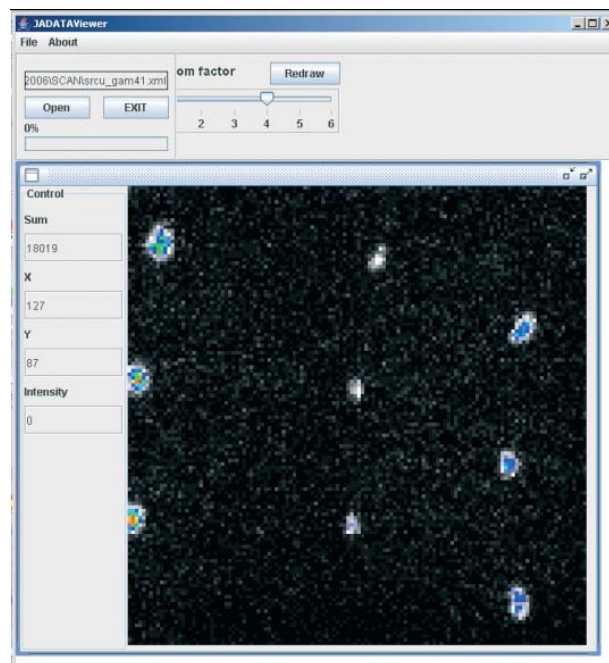

Figure 2. Visualization program window.

Using a long polarizing bender in combination with PSD on 6T2 improve the efficiency of the instrument by approximately a factor of 20-30 compared to the 5C1 diffractometer currently existing at the LLB. This will provide unmatched speed of data collection from very small samples with relatively large unit-cells.

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