NEUTRON DIFFRACTION INSTRUMENTS AT THE BR2-REACTOR AND THEIR USE IN THE STUDY OF CRYSTAL AND MAGNETIC STRUCTURES

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INTRODUCTION

The study of structural properties of condensed matter is frequently performed by means of methods based on X-ray, electron or neutron scattering.

In many particular cases the latter technique offers definite advantages which are mainly based on the following characteristics of neutron-matter interaction.

- The large penetration depth for neutrons in matter (with the exception of a few elements), which allow the study of large samples and the use of wavelengths from 0.5 to 5 Å, and even to 10 Å.
- The absence of an atomic form factor.
- The irregular dependence of the scattering length for the different elements as a function of their atomic number.
- The large cross section for magnetic scattering.
- The energy of thermal neutrons which allows the direct measurement of the energy exchange between the neutrons and the scatterer.

In this contribution three of the four neutron diffraction instruments for solid state research, installed at the BR2 reactor, are first described in detail.

In a second section a short description is given of two cases of structure studies, which have recently been performed in our institute: an illustration of the possibilities of using neutron diffraction in the determination of crystal and magnetic structures.

I. DESCRIPTION OF THE INSTRUMENTS FOR NEUTRON SCATTERING INSTALLED AT THE BR2 REACTOR

1. Instruments for elastic neutron scattering (diffraction)

At the beam port R5 of the BR2 reactor two diffractometers are installed, one for single crystal and one for powder investigations.

In figure 1 a drawing of the installation is shown. The numbers on

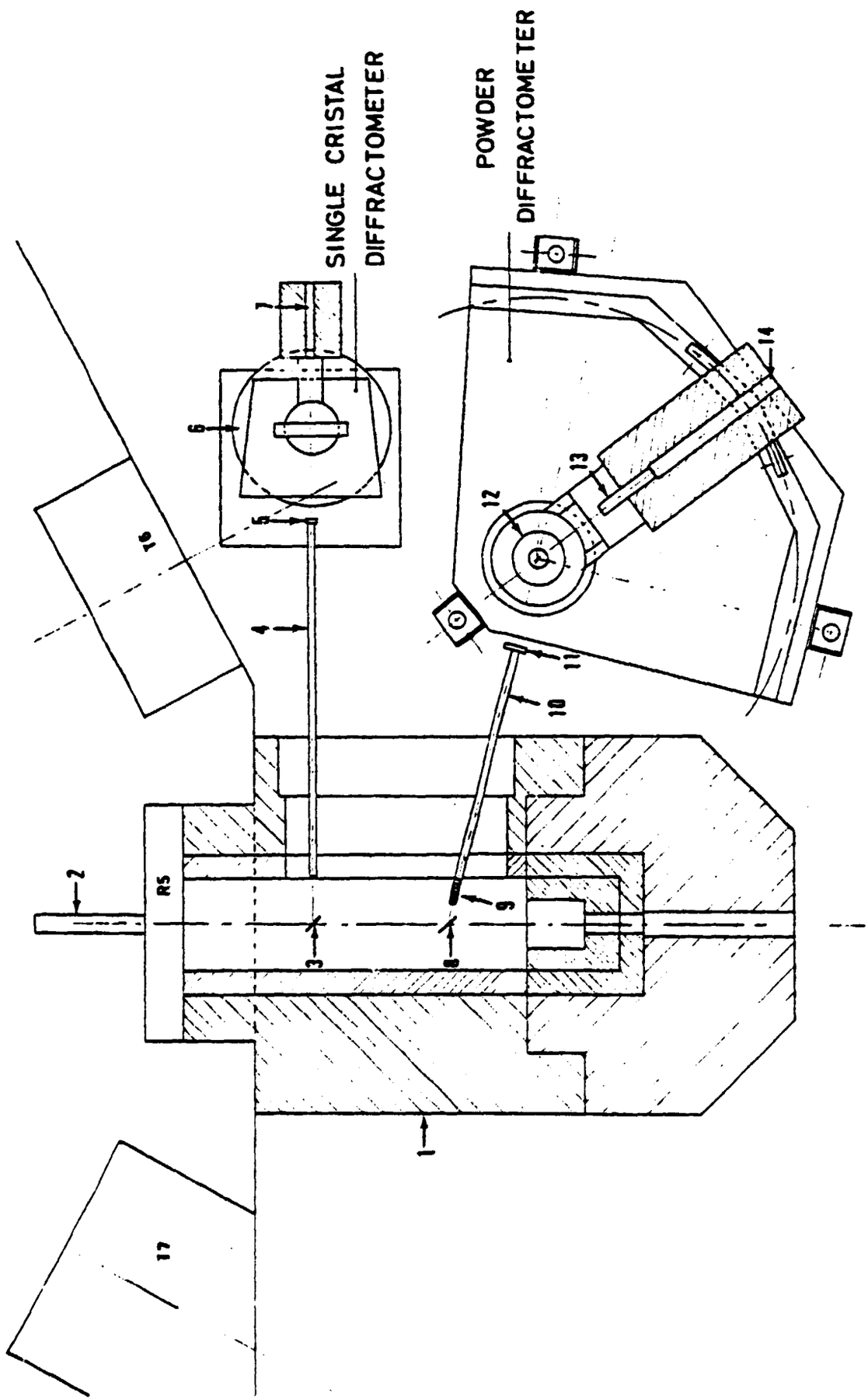


Fig. 1. Experimental set-up for powder and single crystal neutron diffraction measurements installed at beam port R5 of BR2. The numbers refer to the text.

the figure refer to details of the instruments as discussed below.

To stop the direct radiation from the reactor beam a large shielding (1) is built which houses the monochromator crystals. The shielding is composed, looking from the inside to the outside, of 3 cm thick plates consisting of a mixture of B_4C with resin , 10 cm of steel and a fast neutron shielding consisting of a 75 % parafine 25 % borax mixture with thicknesses varying between 50 and 65 cm. In the direct beam a beam catcher of lead and steel stops the gamma radiation from the reactor.

1.1. Single crystal diffractometer

1.1.1. Description of the instrument

From the polychromatic neutron beam, emerging from the reactor, a monochromatic beam is selected by Bragg diffraction on a large single crystal (3). The diffracting planes of this "monocnromator" crystal make an angle of about 45° with respect to the incident beam.

The monochromatic beam falls on a single crystal sample which is mounted on a "four circle" diffractometer (6). The base of the diffractometer is an X-ray instrument from the "Picker" corporation. The "chi" and "phi" rotation mechanisms delivered by the firm "Stoe" have been adapted to the base in our institute. The outer diameter of the chi-circle is 336 mm.

Stepping motors are used to perform the different motions. The diffrectometer is controlled on-line by a PDP8-E computer. This computer calculates the rotation direction and the number of steps to be done by the motors for each (hkl) plane, (the unit cell dimensions and an "orientation matrix" defining the orientation of the single crystal with respect to the spectrometer, being fed in the computer). The number of steps is written in external memories and all motors are moving together. On the drive worm gear axes incremental digitizers are mounted. After each rotation, the number of impulsions counted from the digitizersis compered with the number of impulsions given to the stepping motors. If there is a discrepancy between both, the computer gives a message and corrects for the error which occurred. Up to now the operation of this system is quite satisfactory.

The neutrons scattered by the sample are detected by a BF_3 counter (7) ("Reuter Stokes" type RSN-7), with ceramic end window, boron enriched to 96 % ^{10}B, filling pressure 120 cm Hg, diameter 1 inch and a sensitive length of 8 - 1/8 inch. The limits of the measurable scattering angles are $\pm$ 135°. The shielding around the detector consists, from inside to outside, of a 2 mm thick cadmium sheet, 1 cm B_4C powder and 7 cm parafine.

In the monochromatic beam a monitor (5) is mounted to take account of

the fluctuations in the incident neutron intensity. The monitor is a flat "LND" fission counter with a sensitivity of 1 count per 10^2 neutrons

Before the monochromator (3) a collimator (2) with a cross section of 4 x 4 cm and a length of 1 m is installed resulting in a vertical as well as a horizontal divergence of about 2.3°. The collimator between the monochromator and the sample (4) is also 1 m long and has a square cross section of 1.8 x 1.8 cm reducing the horizontal and vertical divergence to 1°. (The beam cross section may be increased up to 2.8 x 2.8 cm). Cagliotti |1| has shown that the divergences of both collimators should be reversed to get the best resolution in the diffraction spectra. However, since it is easier to change the characteristics of the second collimator (4), this solution has been adopted.

1.1.2. Neutron characteristics

As a monochromator the (331) planes of a copper single crystal are presently used, selecting a wavelength of 1.172 Å as measured with a nickel powder sample. The second order contamination, due to the reflection by the (662) planes is about 1 % of the first order. (This quantity is obtained by measuring the intensities diffracted by the (111) planes of a copper single crystal used as sample, for the first and second order wavelengths). Using the (224) planes of a copper monochromator, a wavelength of 1.043 is selected with a second order contamination of about 0.3 %. The reasons why the second order contamination is negligibly small are that the reflectivity of crystals is proportional with λ^3 |2| and that the associated wavelength falls in the tail of the Maxwell distribution of the neutron spectrum.

The following characteristics are all measured with the Cu (331) monochromator. The neutron flux, measured by gold activation just behind the monitor is about 1.4 x 10^5/(cm^2sec).

To have an idea of the contamination of epithermal and fast neutrons in the monochromatic beam, the epicadmium ratio, i.e. the ratio of the intensities measured with and without a 2 mm thick cadmium sheet placed in the beam before the detector, has been measured.

This ratio is, as measured with the BF_3 counter: 1.3 x 10^{-3}. (No corrections have been made for the sensitivity of the detector as a function of the neutron energy, nor for possible saturation effects).

A background measurement has been performed with open beam but without a sample on the spectrometer and with the BF_3 detector at a scattering angle of 30°. In this way 1200 counts/hour are recorded.

1.2. Powder diffractometer

1.2.1. Description of the instrument

Above the first monochromator, a second beam is extracted from the reactor which falls on a second monochromator (8). The diffracting planes make an angle of 38° with respect to the incident beam.

The spectrometer itself is designed and constructed in our institute. The measurements are performed in "step scanning". The magnitude of the steps may be varied, the smallest step being 1 minute of arc. The maximum error found on the steps, measured with an optical system which itself is precise to ± 1 second of arc, is up to + 15 seconds of arc. These errors are due to the inertia of the heavily shielded detector.

The detector (14) is a BF_3 detector "Reuter-Stokes" type RSN-108 S, with ceramic end window, 2 inches in diameter, sensitive length of $12^{3/4}$ inch, filling pressure 76 cm Hg, boron enriched to 96 % ^{10}B. The surrounding shielding is composed of a 2 mm cadmium sheet, 5 cm B_4C powder and 12.5 cm parafine. The range of scattering angles, which can be covered is from 0 to 100°.

The sample table (12) is mechanically coupled to the motion of the detector in a 1/2 ratio. The table can support a weight of about 1 Ton. This allows us to put directly a magnet, cryostats or ovens on it. It may be worthwhile to mention here that, due to the large penetration depth of the neutrons in matter, the construction of windows for cryostats and ovens is much less critical than when other radiations (e.g. X-rays) are used.

The collimator (2) may be changed from outside: collimators with a horizontal divergence of 30 and of 7 minutes are available. The vertical divergence is for both collimators about 2.9°. The cross section of the beam at this place is 5 cm high and 3 cm wide. The second collimator (10) has no Soller slits, and therefore it has a large horizontal and vertical divergence. However this collimator is of less importance for the resolution characteristics [1]. The cross section of the beam has been reduced here to 3 x 3 cm^2, since the cross section of the available pyrolitic graphite filter (9), used to eliminate the second order contamination, is only 3,5 x 3,5 cm^2. The horizontal collimation of the third collimator (13) can be changed between 20 and 60 minutes of arc by changing the number of steel plates defining the width of the slits.

The monitor (11) is a flat fission counter with a sensitivity of 1 count per 10^3 incident neutrons from "Amperex" type B 300 03.

1.2.2. Neutron characteristics

At this time the (111) planes of copper are used as a monochromator. The measured wavelength is 2.564 Å. In this case the second order contamination is very important. It is filtered out by using a filter of pyrolitic graphite. The transmission characteristics of such a filter are given in the contribution by Dr. M. Nève de Mévergnies in this report. (The first order wavelength corresponds with a neutron energy of 13.5 meV, the second order with about 50 meV). With this filter, the higher order contamination becomes negligibly small (about 0.6 %).

The epicadmium ratio is 3×10^{-4} measured with the BF_3 detector. The better epicadmium ratio measured for the powder diffractometer with respect to the single crystal diffractometer is due to the presence of the graphite filter in the incident beam.

At a scattering angle of 30° for the detector a background of about 450 counts per hour is measured with beam open but without a sample .

1.2.3. Recent developments in the analysis of powder diffraction patterns

Cagliotti et al. [1] have shown that the spatial transmission characteristics of neutron collimators can best be described by a Gaussian distribution. Since the mosaic spread of the monochromator, and of the crystal domains in the grains of the powder sample, have also Gaussian distributions, the line shape of the peaks in the diffracted spectra, which is a convolution of all these Gaussian distributions, will also be nearly Gaussian. This fact has led Rietveld [3] to the idea to use, instead of the integrated intensities which as a rule were used in the function to be minimized in the refinement programs of the crystal parameters, a Gaussian shape for the calculated intensities and to compare point by point; the measured and calculated intensities in the neighbourhood of each Bragg reflection. The big advantage of this "profile analysis" method consists in the fact that the intensity contribution of overlapping peaks in the diffraction spectra are much more accurately used in the minimizing function than can be done when integrated intensities are used. Therefore, the part of the diffraction pattern at larger scattering angles, which was nearly useless in the analysis based on integrated intensities, has regained its full importance and the efforts to improve the resolution of the powder diffractometers at larger scattering angles have again been increased. Hewat [4] made calculations about the optimum resolution conditions. To compensate for the loss in intensity, due to the increased resolution, a multi-counter bank can be installed on the spectrometer [5]. Depending on the number of detectors

pattern installed and on the dimensions of the sample, a complete powder diffraction can be obtained in a time of 24 or 48 hours, even at a reactor with moderate flux.

To conclude one may say that, both for crystal structure determinations and for magnetic structure research the profile analysis method has improved the neutron powder measurements so much that in many cases the studies may be performed on powders where the much more difficult and more time consuming single crystal measurements were necessary before. A good example is the recent Hewat's study of ferroelectric phase transitions in potassium niobate [6].

However, it is good to remember that the profile analysis method is a method for REFINEMENT of the crystal parameters and that it remains necessary to gather as much information as possible with other techniques.

1.3. Remarks concerning future developments

1.3.1. Besides the several monochromators that are presently available (copper, lead, aluminium, zinc and pyrolitic graphite) germanium single crystals will be procurred as monochromators. Germanium crystallises with the diamond structure and therefore it has many crystal planes for which the second order planes have a structure factor equal to zero. However, since such single crystals are generally very perfect, the crystals have to be squashed mechanically to increase the mosaic spread. Such a technique is not yet available in our institute.

1.3.2. The part of the shielding (1), where the collimators (4) and (9) are situated, is composed of compressed wood (permally). By cutting holes in it, with other directions, it is possible to change the diffraction angles of the monochromators. Such changes may, if necessary, be performed in one or two days.

1.3.3. The installation of a detector bank is taken into consideration. Besides the large gain in time for the measurements, the range of the attainable diffraction angles will be increased from 100° to 145°.

2. Instruments for inelastic neutron scattering

2.1. Triple axes spectrometer

This spectrometer is installed at beam tube R4. The main differences of this spectrometer with respect to the diffraction instruments consists firstly in the possibility to very the diffraction angle of the monochromator between some limits, and as a result to change the selected wavelength (and energy) of the neutrons in a continuous way; secondly in the fact that the neutron energies, scattered by the sample, are analysed by Bragg scattering on a single crystal (called analyser crystal).

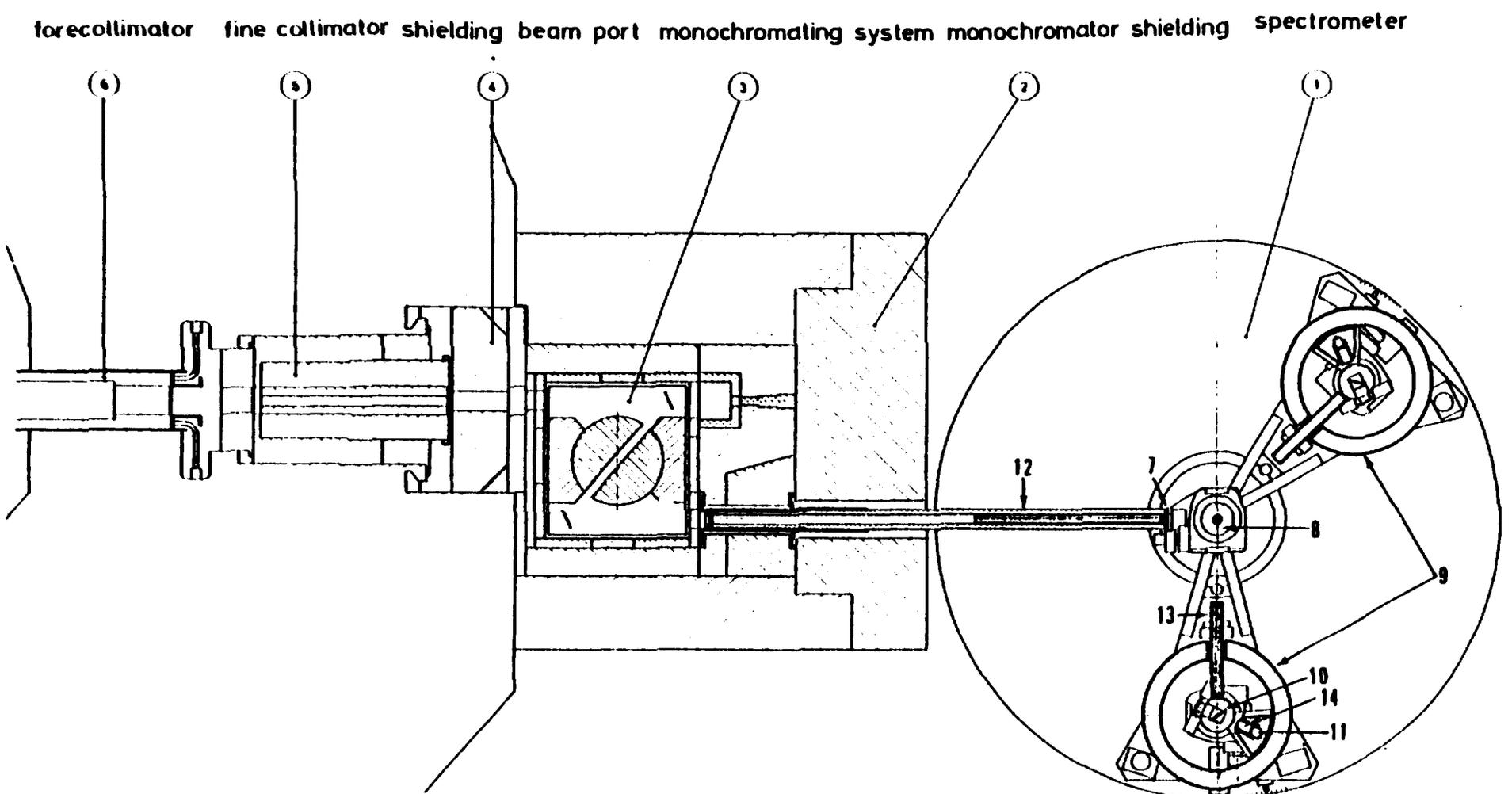


Fig. 2. Design of the triple-axis spectrometer installed at beam port R4 of BR2 reactor. The numbers refer to the text.

2.1.1. Description of the instrument

Figure 2 shows a drawing of the instrument. The shielding (2), to stop the direct beam, has a similar composition as described for the diffractometers. The dimensions of the different parts are slightly larger since the neutron flux at R4 is between 2 to 5 times larger than at beam tube R5.

In this instrument two monochromators (3) are used instead of one. The advantages of using two monochromators may be summarized as follows.

- The contamination of epithermal and fast neutrons (which is quite important at a reactor of the BR2 type) in the monochromatic beam becomes negligibly small.

- The divergency of the twice diffracted beam is smaller than with one monochromator and it is not necessary to use Soller slit collimators in the polychromatic incident beam. Therefore the energy and angular resolution are better than in case one monochromator is used.

- The second order contamination becomes smaller, since the reflectivity at each monochromator is proportional to λ^3.

- The mechanical construction could be realized in the workshop of our institute.

- Since in case one monochromator is used the analysing system AND the sample table have to rotate around the monochromator, the double monochromator system was more favourable in view of the space available near the beam port R4 in the reactor hall.

The big disadvantage, however, of using two monochromators consists in the loss of neutron intensity.

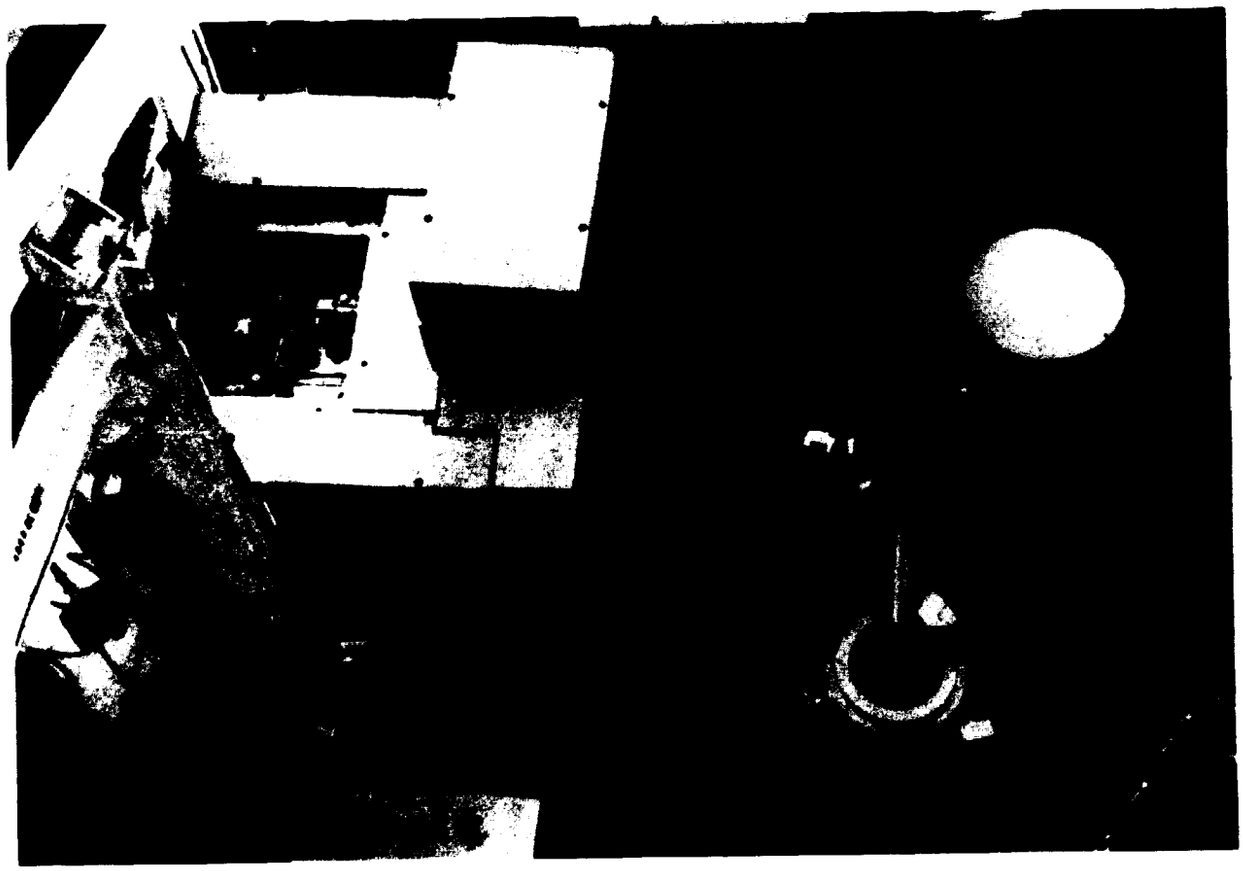
For mechanical reasons the Bragg angles of the monochromators are limited to the range between 25° and 65° (in practice 26° and 64° are used as limits). With two monochromators the change in Bragg angle is obtained with a combination of rotational and translational motion of the monochromators.

As monochromators and analysers, the following crystals are available at this time:

(0002) planes of pyrolitic graphite
Cu(220)
Cu(111)
Cu(511)
Zn(0002)

A flat fission counter is used as monitor (7). It is an "LND" type 3053, with a sensitivity of 1 count per 10^3 neutrons per second. The sample is mounted on the sample table (8).

Fig. 3a. Photograph of the powder and single crystal diffractometers. The powder diffractometer is on the foreground. During the measurements a "plastic-B_4C" plate is put between both spectrometers to screen both instruments from each other.



b. Photograph of the triple axis instrument. The shieldings of one analyser system and above the driving mechanism of the monochromators are removed.

Two analysing systems (9) may be used. They have a measuring range of $\pm$ 135° (without taking into account the interference between both). The analyser crystal is situated at (10). The detector (11) is a ^{3}He counter, filling pressure 4 atm, 2 inch diameter. Around the detector a shielding of 2 mm cadmium and a volume filled with B_4C powder are used. To reduce the background the crystal and detector are screened with a moveable shielding of 10 cm filled with a mixture of 75 % parafine and 25 % borax.

The cross section of all collimators is 5 x 5 cm^2. The collimator in the incident beam (5) is 1 m long but has no Soller slits. The second collimator (12) is evacuated; stainless steel plates can be introduced over a length of 1 m to change the divergency of the beam. Also collimators (13) and (14) have the possibility of variable divergency by inserting more or less stainless steel plates in it.

2.1.2. Some neutron characteristics

The neutron characteristics given below are measured with two Cu(220) monochromators at a scattering angle of about 45° giving a measured wavelength of 1.81 Å. Half of the maximum number of steel plates was present in each collimator. The measurements were done with the analyser and the detector at position zero, no analyser crystal being present.

The epicadmium ratio is about 1 x 10^{-5}.

The background measured with the analyser system at an angle of 30° is about 300 counts per hour.

Fotographs of the diffractometers and the triple-axis spectrometer are shown in figs. 3a and 3b.

2.2. Time-of-flight instrument

This spectrometer for inelastic neutron experiments, is described in the contribution in this report by W. Wegener and S. Hautecler.

3. Remarks concerning the electronics and the use of the PDP8-E computer

3.1. Present use of the computer

The computer was originally equiped with 8 K of core memory, a fast reader-punch and two teletypes for the single crystal diffractometer and the triple axes spectrometer respectively. The control programs are written in assembler language. For each instrument 4 K of core memory is used. The interference time, i.e. the time that the computer is inaccessible for one instrument because it is occupied with the other one, is only a fraction of a second: the time necessary to calculate new positions. For both instruments several measuring routines are available on paper tape. A new routine for one instrument can be read in with the fast reader while the other instrument remains controlled.

The disadvantage of the use of programs written in assembler, instead of using higher programming languages as Basic or Fortran, is largely reduced by the fact that at our institute a central PDP8 computer, equiped with the "OS8" programming system and a line printer is available for the several users of PDP 8 computers (12 at this time). New routines, or changes on existing routines may be worked out and tested on this computer.

The advantage of using teletypes as controls for both instruments is that input can be given and output can be obtained on papertape for both instruments separately.

3.2. Future changes

The core memory of the computer has recently been extended to 16 K. It is the aim to use it also for controlling the powder diffractometer. It is intended to add to the output devices a simple plotter system and a faster access to the big central computer than is possible with punched paper tape, either by direct connection to the computer, or by the addition of an IBM competible magnetic tape.

3.3. Electronic equipment

Most of the electronic equipment has been built in our institute at the neutron physics department. The electronics for the single crystal diffractometer and triple axes spectrometer are built on the basis of the "NIM" system; the electronics of the powder diffractometer is based on the "Camac" system.

4. Auxiliary equipment

All the auxiliary devices described next can be used at any of the four neutron scattering instruments.

4.1. Cryostats

Three cryostats for liquid helium are available. Their main characteristics are summarized below.

4.1.1. Leybold cryostat

- This cryostat is equipped with a device for the condensation of liquids and gases.
- Capacity of the helium vessel: about 12 l.
- Consumption of liquid helium: (depending on temperature and sample holder (e.g. additional temperature sensors)), about 0.3 l per hour.
- Temperature variable between 2.3 K and 300 K.
- Temperature stability (depending on temperature) about 0.01 K.
- Sample dimension: up to 10 cm^2 possible.

Fig. 4a. Crystal and magnetic structure at 4.2 K of Mn_3B_4.
b. Temperature dependence of the magnetic peaks of Mn_3B_4 between scattering angles of 3 - 6°.

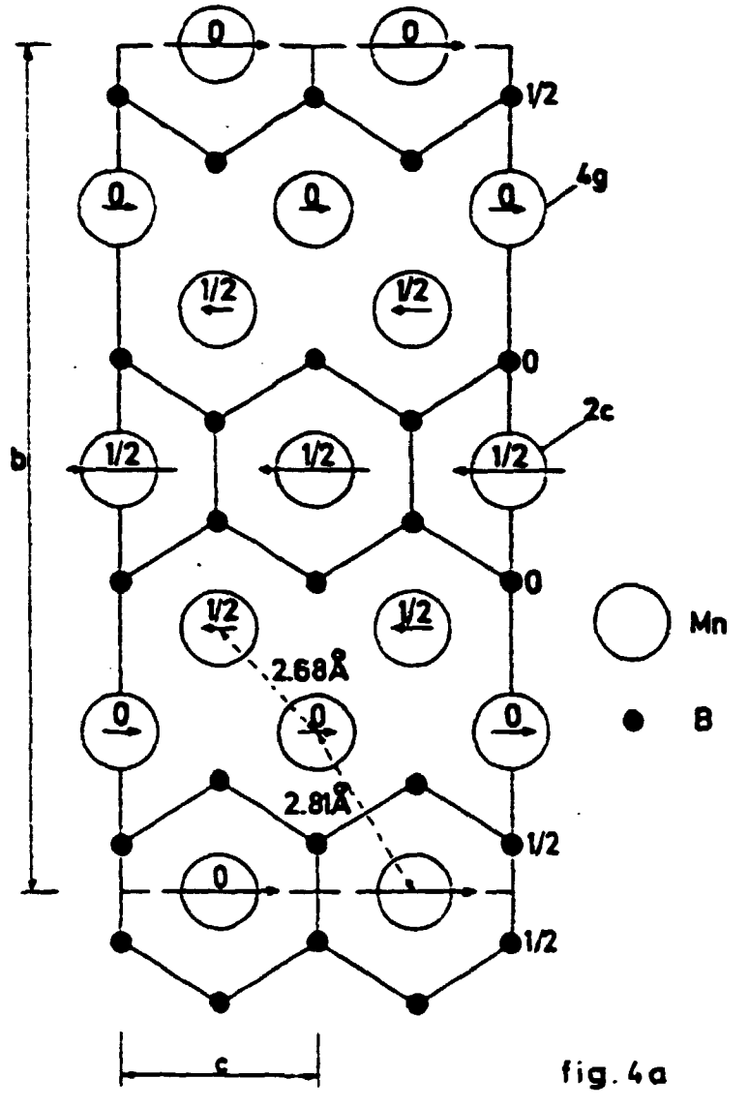


fig. 4a

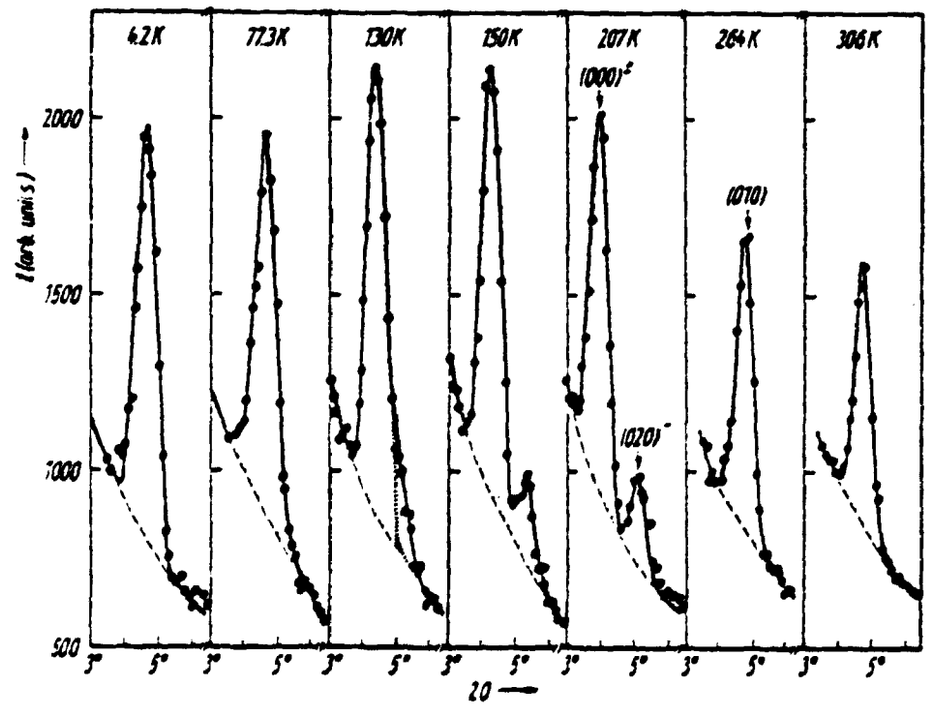


fig. 4b

4.1.2. Cryostat "Oxford Instruments"

- The sample holder and its temperature regulation is interchangeable. These parts are built in our institute.
- Volume of liquid helium vessel: about 8 l.
- Consumption of liquid helium (measured without sample nor temperature sensors), 0.08 l per hour.
- An insert will be procured to mount single crystals in the cryostat. This will allow their orientation at low temperatures from the outside of the cryostat.

4.1.3. Supairco cryostat

The cryostat is normally used without a variable temperature device. In this case the consumption of liquid helium is extremely small: 0.5 l per 24 hours. The contents of the liquid helium vessel is 5 l.

Using liquid nitrogen, temperatures down to 45 K may be obtained by reducing the vapour pressure above the (solid) nitrogen. A device has been built which allows the temperature of the sample to be changed within limits temperature ranges.

4.2. Cryostats for liquid nitrogen

Besides the cryostats for liquid helium, several cryostats for liquid nitrogen are available. They are all designed and built in our institute.

4.3. Liquid helium supply

A "Collins" helium liquefactor is available. However, when large quantities of liquid helium are used, the liquid helium is purchased abroad.

4.4. Ovens

Two ovens for measurements up to about 400°C and 700°C respectively are available.

4.5. Special goniometer heads

Two big goniometer heads are available on which the cryostats and oven may be mounted. This allows to tilt the cryostat or oven over angles of $\pm$ 15° so that some measurements on single crystals may be performed with these devices.

4.6. Magnets

Two magnets are at our disposal. A small one with pole diameter of 8 cm and a fixed interpole distance of 3 cm. Continuous fields up to 6000 Gauss may be obtained.

A larger magnet with pole diameter of 10 cm and variable gap between the poles is also available.

The maximum continuous fields are:

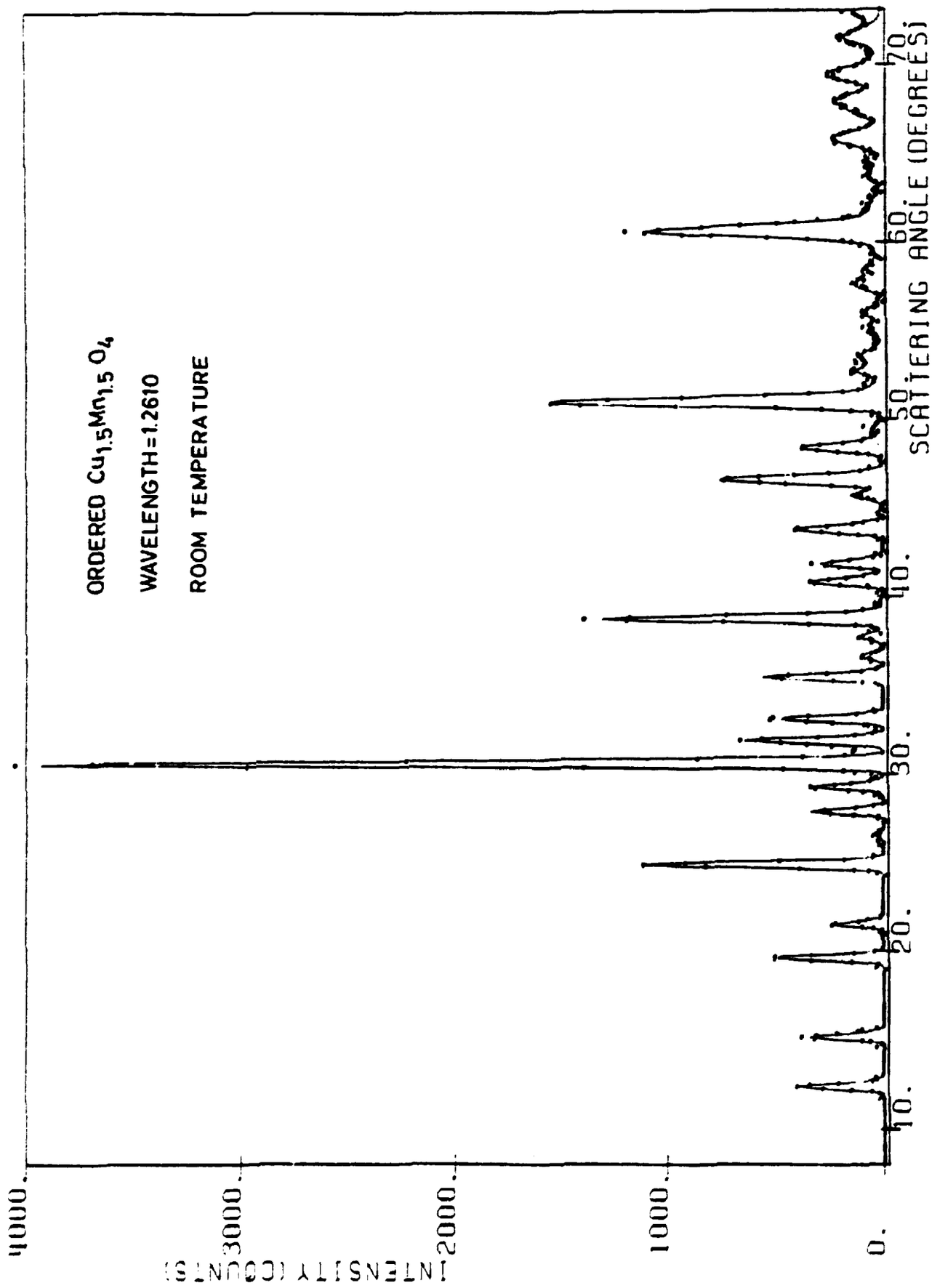


Fig. 5. Profile analysis of disordered $Cu_{1.5}Mn_{1.5}O_4$. The points represent measured intensities, the continuous line corresponds to the calculated intensity at each point.

1.5 cm gap ~ 16 K Gauss

3 cm gap ~ 10 K Gauss

5 cm gap ~ 7 K Gauss

This magnet can be rotated around a horizontal axis. Special tails can be fitted to most cryostats for low temperature measurements in magnetic fields. In that case, however, the larger pole gaps have to be used.

When the field direction of the magnet is used parallel to the scattering vector, the largest scattering angle (Bragg angle of the sample) which may be used with a gap of 5 cm and a beam width of 3 cm is 25 degrees.

II. EXAMPLES OF STRUCTURE DETERMINATIONS

1. Study of the magnetic structure of Mn_3B_4

The phase diagram of the manganese boron system is very complicated and stable mixtures of Mn_4B, Mn_2B, MnB, Mn_3B_4, MnB_2 and MnB_4 are known |7|. The magnetic properties of the different phases have been extensively studied, since some show a ferromagnetic or antiferromagnetic or even a more complex behaviour. Two phases Mn_3B_4 |8| and MnB_2 |9| have been studied with neutrons in our institute since contradictory interpretations, deduced from macroscopic properties, mostly susceptibility measurements, were published. The interpretation of magnetic structure investigations on Mn_3B_4 is hampered by the fact that the manganese atoms are distributed in the unit cell on two different crystallographic sites. The structure is shown in figure 4a. At one site the Mn atoms are surrounded by B atoms, at the other site two layers of Mn atoms are in contact with each other.

From the neutron diffraction measurements the correct magnetic distributions of the magnetic moments over both types of manganese atoms and the magnetic structure could be deduced. Figure 4b shows the behaviour of the (010) magnetic superstructure line as a function of temperature. This line is splitted into two lines in the temperature region between 130 K and 207 K. This could be explained by assuming a spiral structure. With the picture obtained for the magnetic structure, the susceptibility measurements on single crystals |10| could be fully understood.

From this example it is clear that neutron diffraction may yield important information about magnetic structures which can hardly be obtained by other techniques. However, these other techniques remain very useful. For example susceptibility measurements as a function of temperature are much faster and easily yield information about the field dependence of the

magnetic structure as well. Moreover, since also in neutron diffraction models for the magnetic structure are used to explain the measured intensities, these models are sometimes not unique. Therefore information obtained from other magnetic measurements is not only useful but sometimes indispensable to decide which model is the correct one.

2. Study of the crystal structure of spinels

Many compounds crystallise in the spinel structure. The general formula for these compounds is $A[B_2]X_4$. The X atoms are anions and may be oxygen, sulphur or selenium. They have a tetrahedral or octahedral arrangement. A and B atoms represent cations, the A atoms being at the center of the tetrahedral holes, the B atoms at the center of the octahedral ones. There is a large variety of different combinations of cations which form spinels and if different cations are present, ordering effects may appear as well at the A as at the B sites. Because of the important technological applications of these compounds, owing to their magnetic properties, systematic studies have been undertaken since a few years to connect their actual structure, including cation distribution on A and B sites and ordering effects, with the way of preparation.

Such studies are performed in the laboratories of V.A.M. Brabers from the T.H. in Eindhoven and of Professor G. Robbrecht from the R.U. Gent. In collaboration with these laboratories we studied the structure of the spinels $CuMg_{0.5}Mn_{1.5}O_4$, and $Cu_{1.5}Mn_{1.5}O_4$ for different preparation conditions. These structures are very favourable to be studied with neutrons since Mn has a scattering length with opposite sign with respect to the scattering lengths of the other cations so that very accurate results could be obtained [11]. The parameters were further optimized by using the method with integrated intensities. Since a program for profile analysis became available at our institute, we tested the program on one of these measurements. Figure 5 shows the results. The points represent the measured values, the continuous curve the calculated ones. The parameters obtained from the profile analysis are very close to those obtained in the earlier analysis.

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Part of the installation of the diffraction equipment was designed by M. Van Roy and J. Baudeweyns (materials science).

The electronic equipment was designed by E. Mies and P. D'Hooghe (neutron physics department); the interfaces for the PDP8 computer were built by R. Caron (department applied mathematics).

The adaptations to the cryostats and the components for the auxiliary equipment were mostly designed by M. Van Roy, J. Brouwers and J. Baudeweyns. F. Biermans, J. Baudeweyns and A. Hooyberghs took care of the liquid helium supply.

DISCUSSION

White (Grenoble)

Could you tell me what is the fast/slow background at your 3 axis machine ?

Legrand

Due to the double monochromator, used in the instrument, the fast neutron background in the incident beam is very low. Also the general background without sample is low. Some numbers which illustrate this are given in the text.

Wartena (C.B.N.M., Geel)

1) What is the monitor you use in your spectrometer,
2) what is the spatial and the energetic dispersion of your beam after the monochromator ?

Legrand

1) The monitors used are fission counters with a sensitivity of 1 count per 10^2 or 1 count per 10^3 per cm^2 of incident neutrons.
2) Both characteristics depend on the collimation used, the scattering angle of the monochromator, its mosaic spread and interplanar spacing. For the powder diffractometer the collimation of the incident beam as currently used is : $\sim$ 30 minutes of arc horizontally and a few degrees vertically. With the Cu(111) planes and a scattering angle of 37.8 degrees, $\Delta\lambda$ is about 0.03 Å and λ is 2.561 Å.