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CROSSCORRELATION TECHNIQUES USED IN NEUTRON POLARISATION ANALYSIS STUDIES OF STATIC AND DYNAMIC PHENOMENA IN DISORDERED SOLIDS

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Résumé - LONGPOL l'instrument d'analyse des neutrons polarisés, à AAEC Research Establishment, Lucas Heights, Australie, a été modifié pour permettre l'analyse, en temps-de-vol, des neutrons diffusés. La modification utilise la méthode de corrélation dans laquelle la polarisation des neutrons avant la diffusion par l'échantillon est modulée suivant une séquence pseudo-aléatoire. Une demonstration de la méthode est donnée dans laquelle des magnons d'un crystal antiferromagnétique du γ-MnNi ont été observés et isolés de la diffusion élastique diffuse.

Abstract - The LONGPOL neutron polarisation analysis instrument at AAEC Research Establishment, Lucas Heights, Australia, has been modified to allow time-of-flight analysis of scattered neutrons. The modification involves the implementation of a crosscorrelation technique in which the neutron polarisation prior to the scattering sample is modulated according to a pseudorandom sequence. A demonstration of the technique is given in which magnons in an antiferromagnetic γ-MnNi crystal have been observed and isolated from the diffuse elastic scattering.

1. Introduction

For almost ten years a long wavelength neutron polarisation analysis instrument, LONGPOL, has been in routine operation at the HIFAR Reactor, Lucas Heights, Australia. Over this period the instrument has provided a wealth of information on atomic ordering and magnetic moment distribution in spin glass alloys [eg. 1, 2] and disordered antiferromagnets [eg. 3-5]. In addition further experiments have been performed to ascertain the spin dependent neutron scattering cross sections of a number of elements [eg. 6, 7], and also to estimate very low hydrogen impurity concentrations in solids [8].

While such measurements have illustrated the power of polarisation analysis in studies of *static* neutron scattering processes in a variety of materials, the unambiguous separation of the various neutron spin dependent scattering cross sections afforded by the technique is expected to be similarly valuable in examination of *dynamic* scattering processes. For this reason the original LONGPOL instrument, which has been described in detail elsewhere [9, 10], has recently undergone some modifications, which include the provision for time-of-flight analysis of the scattered neutrons, extending the scope of possible measurements to both static and dynamic scattering. The purpose of this paper is to provide a brief description of the modified LONGPOL and to present a preliminary measurement obtained using full time-of-flight analysis.

2. LONGPOL: Experimental arrangement

A schematic diagram of LONGPOL is shown in figure 1. Thermal neutron beam monochromation is obtained using a double crystal "dog-leg" monochromator consisting

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of two oriented pyrolytic graphite crystals (Union Carbide, grade ZYH) with mosaic spread of 3.5° ± 1.5° FWHM. The (002) reflection is used to select neutrons of

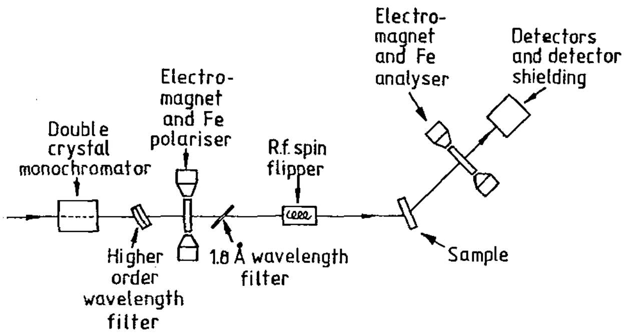

Figure 1. *Schematic diagram of the LONGPOL instrument*

wavelength 3.6Å, the resulting beam having a FWHM spread of 0.3Å. At 3.6Å the sacrifice of wavelength resolution for intensity is a necessary one. However, as LONGPOL is used primarily for diffuse scattering studies, the broad wavelength resolution does not pose a serious problem. A problem does arise, however, from the higher order wavelength contamination of the incident beam. The $\lambda/2$ component of the beam is reduced by a further 3.5° mosaic pyrolytic graphite crystal, while a number of 5° mosaic crystals are tuned to attenuate the third and higher order contamination.

The method of neutron polarisation on the present LONGPOL is unchanged from that of the original instrument and a detailed description and analysis of the method can be found in references 9 and 10. Briefly, polarisation of the incident monochromatic beam and spin analysis of the scattered beam are achieved by transmission of neutrons through magnetically saturated 6mm thick polycrystalline iron filters. With these filters measurement of beam polarisation using the double transmission effect yields a value of 42%. The improvement in polarisation over the original LONGPOL, which had a measured value of 33%, is mainly due to the tighter wavelength resolution of the present instrument. [Previously the incident beam had a wavelength spread of 0.6Å FWHM].

The polarising and analyzing filters are magnetised in the same direction allowing only those neutrons that undergo non spin flip (NSF) scattering at the sample to be detected. Spin flip (SF) scattering is observed by activating a neutron spin flipper positioned before the sample. The spinflipper currently used on LONGPOL is a 500kHz radiofrequency coil, 50mm long, within a uniform tunable dc magnetic field. The measured flipping efficiency is 98% ± 3%.

At the sample position the incident beam is 25mm in diameter and the polarisation of the beam is directed along the scattering vector for elastic scattering in the horizontal plane. Scattered neutrons are counted by a group of three 25mm diameter 4 atmosphere, ^{3}He detectors.

3. Time-of-flight analysis on LONGPOL

When used in the mode described above, LONGPOL measures separately the *total* NSF and *total* SF scattering from a sample. To perform a full energy analysis of the scattered beam, or to allow discrimination against those neutrons scattered inelastically, a time-of-flight analysis based on the crosscorrelation techniqueis used. On LONGPOL a modification to the conventional crosscorrelation procedure has been implemented wherein the net spin direction rather than the intensity of the incident neutron beam is modulated according to a pseudorandom sequence. Such a modification was first suggested by Mezei and Pellionisz [11] who considered its application to the case of a polarised neutron spectrometer. The mathematical and experimental details of the extension of the polarisation modulated crosscorrelation technique to the case of a polarisation analysis instrument will be presented in detail elsewhere; here it will be sufficient to quote the principle results.

Polarisation modulation of the incident neutron beam before the scattering sample is accomplished by switching the neutron spinflipper on and off using a finite and repeating binary string of L bits, s_i, such that $s_{i+L} = s_i$. Of the L bits of the string K are 1 and L-K are 0. The duty cycle of the string is defined as c, with

$$c = \frac{K-1}{L-1}$$

For the string to be pseudorandom it must have an autocorrelation function A_k such that

$$A_k = \sum_i^L s_i s_{i+k}$$

with $A_k = K$ if $k = 0, L, 2L\ldots$ and $A_k = cK$ otherwise.

Although the binary string is used to drive the spinflipper switching, the actual modulating sequence of the polarisation is a convolution of this statistical base with the transfer function of the spinflipper electronics, $\Gamma(t)$, ie.

$$M(t) = \sum_i s_i \, \Gamma\,(t-t_i) \qquad \text{with } 0 \leq M\ t) \leq 1$$

Ideally Γ (t) should have as rapid a rise and fall time as possible and also be symmetrical such that

$$\sum_i \Gamma\,(t-t_i) = 1 \qquad \text{for all t}$$

At the detector two neutron countrates are measured simultaneously, one arising from the "flipper-on" pulses, the associated neutrons having sampled the SF time-of-flight spectrum of the sample, $S(\tau)$, and the other arising from the "flipper-off" pulses with the associated neutrons sampling the NSF spectrum, $N(\tau)$. In addition there will be an uncorrelated time independent neutron background, b'. The total countrate at time t, Z(t), is therefore

$$Z(t) = Z_{on}(t) + Z_{off}(t) + b'$$

where

$$Z_{on}\,(t) = \int S(\tau') \sum_i s_i \, \Gamma\,(t-t_i-\tau')d\tau'$$

$$Z_{off}\,(t) = \int N(\tau') \sum_i (1-s_i) \, \Gamma\,(t-t_i-\tau')d\tau'$$

If the pseudorandom sequence has been repeated r times in the course of an experiment the final crosscorrelation, $C(\tau)$, will be

$$C(\tau) = \sum_{j=1}^{rL} s_j Z(\tau+t_j)$$

This can be expanded to give, for the crosscorrelation function,

$$C(\tau) = rK(1-c) \int D(\tau')\,\Gamma(\tau-\tau')d\tau' + rKc \int S(\tau')d\tau' + rK(1-c) \int N(\tau')d\tau' + rKb'$$

where $D(\tau')$ is the difference between the "flipper on" and "flipper off" time-of-flight spectra, ie.

$$D(\tau') = S(\tau') - N(\tau')$$

Generally the countrate Z(t), and ultimately $C(\tau)$, will be contained in a finite number of channels, N, of a multichannel analyser. The time width of each channel, δ, is chosen such that $N\delta$ is somewhat greater than the overall time width of both $S(\tau)$ and $N(\tau)$. The background per channel is thus $b = \delta b'$. Using a subscript notation rather than arguments to denote quantities measured in channels of width δ, and also adopting a convention in which asterisk superscripts indicate that a quantity has been convoluted *once* with the pulse shape, $\Gamma(t)$, eg.

$$D^*_\tau = \int_{\tau-\delta/2}^{\tau+\delta/2} \int D(\tau')\, \Gamma(\tau-\tau')d\tau' d\tau$$

the final crosscorrelation can be written as

$$C_\tau = rK\left[(1-c)D^*_\tau + \frac{c}{p}\sum_{\tau=1}^{N} S^*_\tau + \frac{(1-c)}{p}\sum_{\tau=1}^{N} N^*_\tau + b\right]$$

where p is an integer representing the ratio of the modulating pulse width to the channel width, δ. This equation contains all the information embodied in a polarisation modulated crosscorrelation experiment. It can be seen that the result of crosscorrelating the measured countrate with the pseudo random binary string used to switch the spin flipper, yields, in a particular channel τ, a term proportional to the difference between SF and NSF transfer functions of the sample superimposed upon a "background of ignorance" which, within statistical accuracy, should be completely independent of channel.

On LONGPOL the crosscorrelation is performed on-line in a manner similar to the "inverse time-of-flight" method described by Hiismaki [12]: Rather than storing scattered neutron countrates in a multichannel analyser (MCA) according to their times of arrival at the detector and finally cross correlating the stored countrates with the pseudorandom sequence, a detected neutron triggers a sweep of the MCA during which elements of the *delayed* pseudorandom sequence (ie. previous states of the spinflipper) are stored in the appropriate MCA channels. In this way a crosscorrelation pattern, mathematically indentical to C_τ given above, is constructed dynamically. In this mode it is not necessary for the pulse sequence to be pseudorandom and other experiments have been performed with non repeating random sequences.

Pseudorandom switching of the spinflipper is accomplished using a shift register sequence generator which allows the choice of both sequence length ($L = 2^n-1$, with n=1, 2....12) and operating frequency (1 kHz to 100 kHz). The duty cycle of shift register sequences is always $C=\frac{1}{2}$.

4. Aplication of the polarisation modulated crosscorrelation technique

4a. Full time-of-flight analysis An illustration of the application of the LONGPOL time-of-flight facility is given in Figure 2 where a spectrum obtained from an antiferromagnetic γ-MnNi single crystal is shown. The crystal, maintained at room temperature, was oriented such that a low wavevector magnon could be observed. Details of the experimental parameters are given in the figure. The illustrated spectrum was collected in 90 hours, but the position of the magnon was quite clear after 40 hours. For clarity the "background of ignorance" has been subtracted from C_τ leaving a difference spectrum proportional to $D^*_\tau = (S^*_\tau - N^*_\tau)$. No correction has been made for imperfect beam polarisation.

As the polarisation direction of the beam is closely parallel to the scattering vector for small energy changes S^*_τ represents predominantly magnetic scattering whereas N^*_τ is predominantly nuclear scattering. It is therefore to be expected that D^*_τ is negative, as observed, for elastic scattering as, for the present orientation of the crystal, the elastic scattering consists of diffuse atomic disorder and magnetic defect scattering in the ratio ~3:1 [5]. The positive peak at an energy transfer of 10meV, on the other hand, unambiguously shows that at this energy transfer the magnetic scattering is far greater than any nuclear contribution. This peak can therefore be identified as resulting from magnon annihilation.

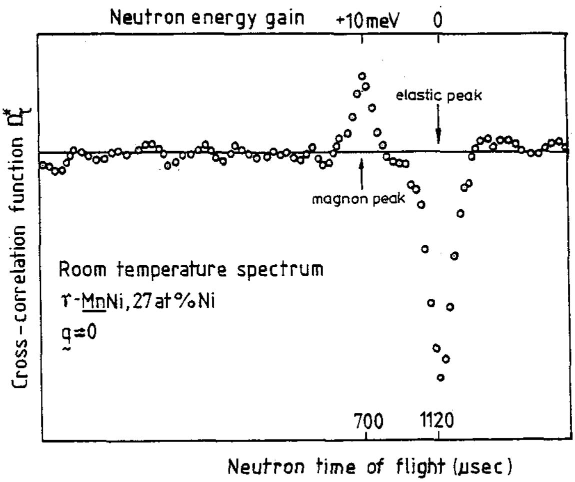

Figure 2. *Time-of-flight spectrum from γ-MnNi (channel width = 25 μsecs, sequence length, L = 4095, duty cycle, c = 0.5, p = 2)*

4b. Discrimination against inelastic scattering: To discriminate against inelastic scattering events the pseudorandom spinflipper switching sequence is delayed by the time-of-flight of elastically scattered neutrons, τ_{el}, and used to trigger an electronic gate routing detected neutrons to one of two scalers depending upon the state of the switching sequence. This is equivalent to evaluating the cross correlation function, C_τ, at a single channel corresponding to $\tau=\tau_{el}$, the channel width being the same as the switching sequence pulse width (ie. p=1). Again the spinflipper switching is controlled by a shift register sequence generator with $c=\frac{1}{2}$. Inspection of the expression for C_τ shows that for the scaler associated with the flipper-on condition

$$C^{on}_{\tau_{el}} = rK\left[\tfrac{1}{2}(S^*_{\tau_{el}} - N^*_{\tau_{el}}) + \tfrac{1}{2}\sum S^*_\tau + \tfrac{1}{2}\sum N^*_\tau + b\right]$$

ie. $$C^{on}_{\tau_{el}} = rK\left[S^*_{\tau_{el}} + \tfrac{1}{2}\left\{\sum S^*_\tau - S^*_{\tau_{el}} + \sum N^*_\tau - N^*_{\tau_{el}}\right\} + b\right]$$

As the total, flipper-on plus flipper-off, inelastic scattering I* can be expressed as

$$I^* = \sum(S^*_\tau + N^*_\tau) - S^*_{\tau_{el}} - N^*_{\tau_{el}}$$

the flipper-on scaler records

$$C^{on}_{\tau_{el}} = rK\left[S^*_{\tau_{el}} + \tfrac{1}{2}I^* + b\right]$$

In this mode, the situation for the flipper-off state is symmetrical with that for the flipper-on and in the other scaler

$$C^{off}_{\tau_{el}} = rK\left[N^*_{\tau_{el}} + \tfrac{1}{2}I^* + b\right]$$

is measured. In other words the elastic flipper-on or flipper-off scattering is measured in the appropriate scaler, while the *total* flipper-on plus flipper-off inelastic scattering is, within statistical accuracy, equally distributed between the two scalers. The difference between the two scalers is, of course, independent of any inelastic scattering processes. The switching frequency of the flipper governs the resolution of the elastic discrimination.

LONGPOL has been used in this mode to assess the elasticity of the neutron scattering in a number of previous experiments [see, eg. 2-8].

5. Summary

In this paper a brief description of the modified LONGPOL neutron polarisation analysis spectrometer has been presented. Particular attention has been paid to the polarisation modulated crosscorrelation technique which is now used on LONGPOL both to provide full time-of-flight analysis of scattered neutrons and to discriminate against inelastic scattering processes in studies of static phenomena. It is expected that, in its present configuration, LONGPOL will continue to provide valuable information on static atomic and magnetic defect scattering while also permitting detailed examination inelastic scattering processes in situations where the unambiguous separation of the various neutron spin dependent scattering cross sections is essential.

A complete description of the LONGPOL instrumentation will be published elsewhere.

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