ICANS-VI
INTERNATIONAL COLLABORATION ON ADVANCED NEUTRON SOURCES
June 27 - July 2, 1982

DYNAMIC RANGE ASPECTS OF PULSED SOURCE INSTRUMENTS

F. Mezei

Institut Laue-Langevin, 156X, 38042 Grenoble, France

ABSTRACT

In recent applications of neutron scattering the dynamic range is found to be an important aspect of instrument performance along with neutron flux and resolution. It is pointed out that due to the inherent use of a broad wavelength band, certain instruments, like small angle scattering and neutron spin echo spectrometers, provide better dynamic range capability on a pulsed source than on a continuous source.

DYNAMIC RANGE ASPECTS OF PULSED SOURCE INSTRUMENTS

F. Mezei

Institut Laue-Langevin, 156X, 38042 Grenoble, France

1. INTRODUCTION

Neutron scattering instruments are most often considered from the double point of view of resolution and neutron intensity only. The fundamental importance of a third parameter, dynamic range (DR), has only been recently realized. This is probably due to the fact that classical neutron scattering instruments have a rather small DR, typically between 1:20 and 1:50 (in what follows DR is characterized by the ratio of the smallest and biggest value of a parameter which can be measured by a given instrument in a single configuration). In recent small angle neutron scattering (SANS) and inelastic (mostly magnetic) studies it has been found, that in order to cover a range wide enough to produce a complete set of data, the same sample had to be investigated in a sequence of similar experiments with different resolutions. Practice has also shown that the wide DR, which was made available for the first time by the rather recent neutron spin echo (NSE) method (about 1:1000) is a most essential feature in some experiments.

In what follows I will discuss experimental examples in order to show that large DR can be crucial in obtaining model independent information, which is the major advantage of neutron scattering. It will also be pointed out that the use of a broad wavelength band on pulsed source instruments is instrumental for achieving an improved DR. This makes pulsed neutron sources particularly well adapted to SANS and quasielastic NSE experiments.

2. EXPERIMENTAL CONSIDERATIONS

The main advantage of neutron scattering with respect to other microscopic methods of probing atomic structure and dynamics is that neutrons can provide model independent information. The neutron scattering cross section is directly related to the correlation function $S(\vec{q},\omega)$ and by neutrons we can explore both space and time via the largely independent experimental parameters $\vec{q}$ and ω. In magnetic problems neutrons present a further unique feature, viz. their direct coupling to the magnetization allows to single out unambiguously the magnetic scattering effects (eventually by the use of polarization analysis).

The a priori model independence of the neutron scattering data is just due to the fact that both parameters $\vec{q}$ and ω are kept track of. In experiments like NMR, ESR, μSR, etc. certain points or integrals in the $(\vec{q},\omega)$ parameter space are only explored. This is why in most cases these data can only be interpreted by fitting to specific models.

However, neutron scattering provides model independent information only if the experimental conditions are good enough that the data reduction does not imply deconvolution or heavy corrections (e.g. for inelasticity in diffraction work). In practice this means sufficient resolution and dynamic range. A parameter we wish to determine often varies substantially e.g. as a function of temperature or over the $(\vec{q},\omega)$ space. If we have to use several instruments to follow this variation, we might face very serious difficulties in patching together the bits of information. In particular, the comparison of absolute scattering intensities from one instrument to another is always a problem. Therefore it is preferable to use instruments with a wide DR in a single setting. This of course implies high resolution on the one end of the range. As a matter of fact, a roughly constant relative resolution ($\delta x/x$=const. over the range of the parameter x) is the best compatible with large DR.

To proceed let us consider a few typical experimental examples. In Fig. 1 the distribution of neutron intensity scattered by Southern beam mottle virus in H_2O solution is shown [1]. These data could not be obtained in a single scan using the D11 SANS instrument at the ILL, because too wide ranges had to be covered both in intensity and momentum transfer. In fact this figure has been assembled from results of several experiments made on different samples, at different neutron wavelengths and using different instrumental configurations. This procedure is tedious, takes longer time than a single scan and it is less reliable, of course.

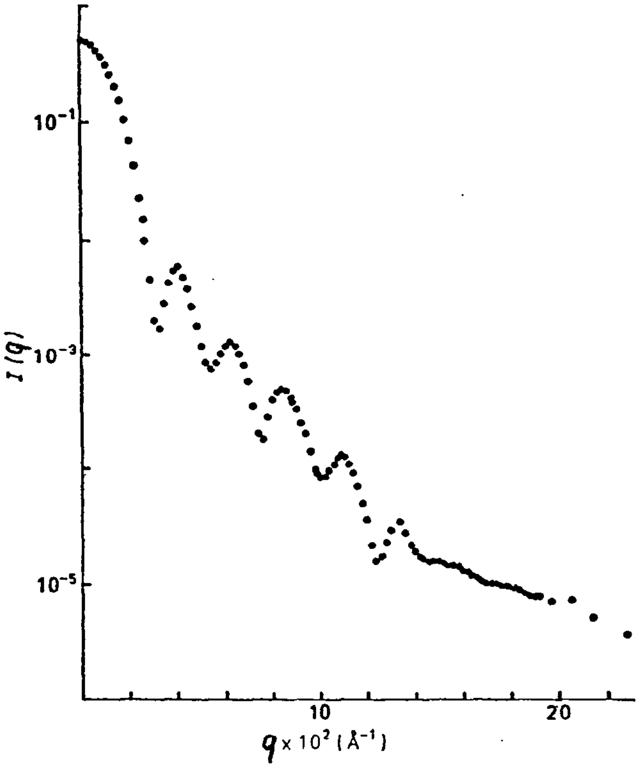

Fig. 1 Neutron intensity distribution scattered by Southern bean mottle virus in H_2O solution as a function of the momentum transfer [1].

The second example (Fig. 2) shows the q dependence of the inelastic Lorentzian line width Γ_q of the critical scattering of iron at the Curie point [2]. It is seen that the results follow the predicted power law $\Gamma_q \alpha q^z$ with $z \simeq 2.5$ over an impressive range of four orders of magnitude in ω. This is in constrast to the interpretation given to anomalies observed in hyperfine field experiments [3], according to which below $q \sim 0.05$ $\mathring{A}^{-1}$ a cross over should take place to the $\Gamma_q \alpha q^2$ behavior. Previous neutron scattering results [4,5] only covered q values above 0.05 $\mathring{A}^{-1}$, and only recent high resolution time-of-flight (TOF) and NSE experiments [2] (made respectively on the IN5 and IN11 instruments at the ILL) allowed to rule out the hypothesis of a crossover, and to give another explanation for the hyperfine field anomalies. The value of the exponent z, however, could only be determined with a precision of ± 0.05 in view of the uncertainties of comparing data taken under different conditions and by different methods. In order to check finer details of theoretical predictions we should determine

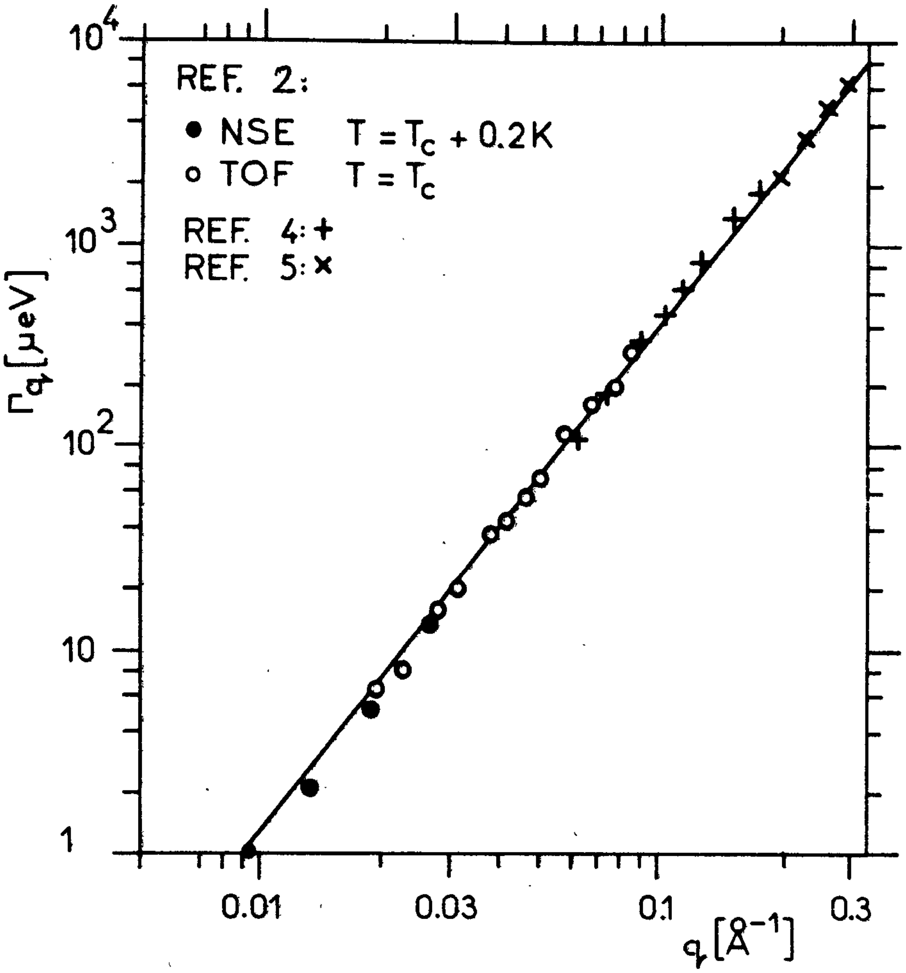

Fig. 2 Momentum dependence of the quasielastic linewidth of the critical scattering of Fe at the Curie point. The recent TOF and NSE results, Ref. [2] were obtained at the ILL, the previous results, Refs. [4] and [5], represent triple-axis data.

z with ± 0.02 precision, which could only be made in a single scan. This example illustrates that (a) the nature of certain physical phonomena makes wide DR experiments indispensable, (b) by using indirect probes (like hyperfine field interaction in this case) it is eventually possible to show if a model assumption works or not, but it is impossible to interpret unambiguously observed deviations from a model and (c) high resolution is necessary in order to achieve large DR.

One last example illustrates that single, large DR scans are indispensable in studying unknown lineshapes. The dynamics of spin relaxation in spin glasses is characterized by an anomalous decay of the spin correlations as a function of time, i.e. by deviations from the usual ext$(-\gamma t)$ form [which leads to the common Lorentzian line shape, $\gamma/(\gamma^2+\omega^2)$, by the $t \to \omega$

Fourier transformation]. This has been established in the pioneering work of Amir Murani [6], who patched together data taken on the IN4, IN5 and IN10 spectrometers at the ILL in order to cover the ω range of 1 μeV to 2 meV. However, this procedure did not allow to obtain quantitative results on the actual lineshape. This was only made possible by using the NSE method, which allowed to cover a 1:600 range in a single scan, incidentally, directly in the time domain [7]. The results [8] in Fig. 3 show that at some temperatures (viz. 30 and 36 K) the data are compatible with the predicted const - ℓn(t) shape (which would give straight lines in the log-scale figure), but not at other temperatures. In this particular case a.c. susceptibility data allowed to extend the results [10] over an improbable range of $1{:}10^{12}$, which revealed that there can be interesting details only apparent on such a large DR (e.g. the drop in the 26K curve between 10^{-8} and 10^{-5} sec). Note that the ESR and μSR experiments made on the same system were invariably evaluated under the obviously wrong assumption of exponential decay. This shows again the fundamental role of neutron scattering as model independent probe.

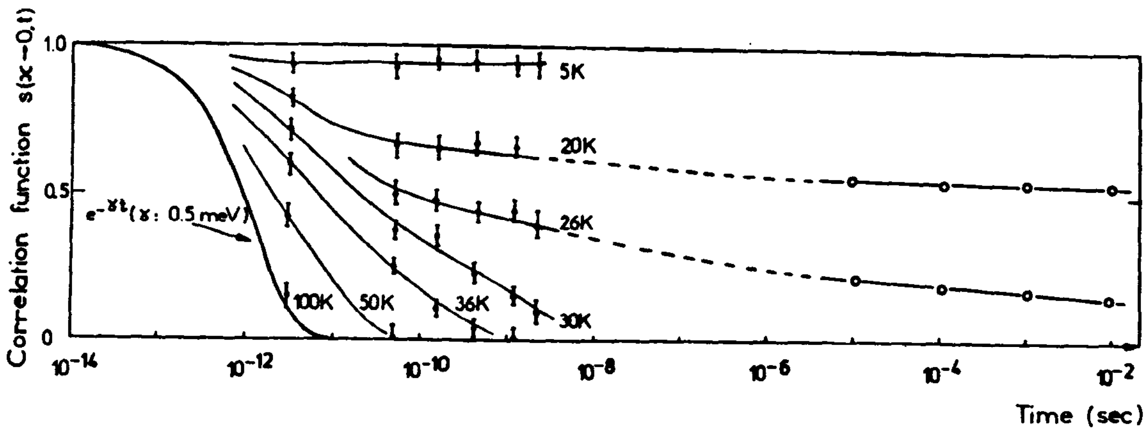

Fig. 3 Decay of the spin-spin correlations vs. time in Cu-5% Mn spin glass alloy. Dots with error bars represent NSE and polarization analysis data (Ref. [8]) measured at $q=0.1$ Å^{-1}. The open circles give values calculated from a.c. susceptibility data (Ref. [9])

3. DYNAMIC RANGE OF PULSED SOURCE INSTRUMENTS

There are basically two ways of making wide DR experiments:

a) use of very high resolution

b) use of several wavelengths

The only existing neutron scattering technique which provides large DR at fixed wavelength by its high resolution capability is NSE with a DR of about 1:1000. Further increase of the range in NSE, and achieving anything like 1:200 - 500 with the other methods requires the application of several wavelengths in a single experiment. This is exactly what pulsed source instruments do, and in what follows I will consider this aspect for SANS and NSE.

The resolution in SANS experiments is determined by the definition of the scattering angle and of the neutron wavelength λ. Since in cold moderators the neutron pulse length is roughly proportional to the wavelength, an approximately constant relative resolution $\delta\lambda/\lambda$ will be maintained in the most interesting part of the wavelength band between about 2 and 10 Å. Note that this resolution happens to be around 1-2%, which is considerably better than what is usually required and used in SANS experiments (viz. about 10%). At any given scattering angle, the smallest q information will be given by the $\lambda \sim 10$ Å neutrons, while the shorter wavelength, higher flux portion of the spectrum provides information at higher q's, where the scattering cross section tends to be smaller (cf. Fig. 1). This intensity compensation effect is a very important feature, and it can make useful much of the data collected during the same time. In usual, fixed wavelength SANS experiments long wavelength is used to access the smallest q values, and thus the measuring time is determined by the low cross section higher q data, taken at the same lower incoming flux. Thus a SANS instrument not only covers a wider DR on a pulsed source than on a continuous one (typically 1:200 compared with 1:40), but also collects data more efficiently. At the final end the data rate at a pulsed source should be comparable to that at a continuous source with a flux about 20-50 times higher than the time averaged pulsed flux.

Many of the above considerations apply to the use of NSE on a pulsed source [11]. The DR could be extended to 1:10000 by using a wavelength band between 3 and 10 Å, which can be handled by supermirror neutron polarizers. In experiments like the study of diffusion at small scattering angles, the above intensity compensation arguments also apply, and in addition a similar situation holds for the resolution. Shorter wavelength neutrons provide information at high q, where the quasielastic linewidth tends to be bigger (cf. Fig. 2), i.e. less resolution is required. In addition, shorter wavelength might even be necessary in order to keep the scattering triangle close to a constant q configuration. (e.g. in Fig. 2 the TOF data could not be extended to higher q values because the inelasticity would have become comparable to the incoming neutron energy of 0.8 meV). For the rate of data collection in NSE at a pulsed source the same figures should apply than those given above for SANS.

4. CONCLUSION

Recent experience shows that in some neutron scattering studies the dynamic range of the instrument used is as important as neutron intensity or resolution. This implies, that the same way as e.g. high flux can not make up for poor resolution, the use of several instruments with different ranges can not always replace a large DR scan in a single setting of a single instrument. Pulsed source instruments are bound to provide superior DR with respect to continuous source machines, due to the inherent use of a broad wavelength band. In particular this feature makes pulsed sources well adapted for small angle scattering and quasielastic neutron spin echo experiments. In these cases the data collection rate corresponds to that on a continuous source with 20-50 times the time averaged flux of the pulsed source, and no good time-of-flight resolution is required, i.e. cold neutron pulses of several 100 μsec length are perfectly acceptable.

REFERENCES

[1] See B. Jacrot Rep. Prog. Phys. 39, 911 (1976)

[2] F. Mezei, to be published.

[3] L. Chow, C. Hohenemser and R. M. Suter, Phys. Rev. Ltr. 45, 908 (1980)

[4] M. F. Collins et al., Phys. Rev. 179, 952 (1969)

[5] S. Boronkay and M. F. Collins, Int. J. Magn. 4, 205 (1973)

[6] See A. P. Murani, J. de Physique Suppl. Coll. 39, C6-1517 (1978)

[7] See Neutron Spin Echo, edited by F. Mezei, (Lecture Notes in Physics, Vol. 128, Springer Verlag, Heidelberg, 1980)

[8] F. Mezei and A. P. Murani, J. Magn. Magn. Mat, 14, 211 (1979)

[9] J. L. Tholence, Solid State Comm. 35, 113 (1980)

[10] F. Mezei, in "Recent Developments in Condensed Matter Physics", Y. T. Devreese, editors (Plenum Press, New York, 1981) pp. 679-694

[11] F. Mezei, Nucl. Inst. Meth., 164, 153 (1979)