

TEST OF A CORRELATION CHOPPER AT A PULSED
SPALLATION NEUTRON SOURCE*

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1. Introduction

The use of correlation time-of-flight techniques at steady-state neutron sources is well established,¹ and has proved to be highly effective in certain extreme situations, for example, highly absorbing samples such as liquid helium-3.² In a typical use of this method, a conventional chopper with one pulse per revolution is replaced by a chopper or other device providing a pseudo-random sequence of pulses. Used either with a white beam (for diffraction), or with a beam monochromated with a crystal analyzer (for inelastic scattering), the conditions of the experiment are essentially unchanged, except that the duty cycle is increased by a factor of order N, where N is the number of pulses produced over the period T of the conventional chopper. Because the different data points in the experimental spectrum after analysis have

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correlated errors, the statistical gain is in general less than N but may still be appreciable in certain circumstances.¹

With a pulsed source, the conventional chopper has the primary function of monochromating the beam rather than pulsing it (although it may also have the function of sharpening the pulse in time). In this case, the replacement of the conventional chopper by a pseudo-random pulsing device has the effect of providing a sequence of measurements at different incident velocities, i.e., different incident energies. The statistical comparison in this case becomes less straightforward because the resolution of each measurement is different. An estimate of the gain factor therefore involves an assessment of the range of incident energies over which the data remains useful, and of the relative value of redundant data taken with different resolution and statistical accuracy at different incident energies. Nevertheless, it appears that the method should be favorable in certain cases,³ similar to the situations (low signal/background, high peak-signal/average-signal) where correlation techniques are favorable in the steady-state situation. At least one demonstration of a statistical chopper in a pulsed beam has been carried out, in this case at a pulsed reactor.⁴

In addition to providing an efficient measurement of the inelastic scattering function $S(Q,E)$, this technique could be valuable in measurements of the elastic structure factor $S(Q,0)$ of amorphous or disordered crystalline solids, by providing an energy analysis which selects the elastic scattering out of the total structure factor $S(Q)$.⁵

In view of these considerations, it seemed worthwhile to carry out a feasibility test of the technique at IPNS. Due to the restricted beam time available for this measurement, shortened further by an unforeseen accelerator breakdown, the data obtained during this test are very limited. Nevertheless, some spectra were obtained and analyzed

successfully, establishing the feasibility of the technique and providing some indication of its usefulness and limitations at a pulsed spallation source.

2. Principle of the Method

The method is already discussed at length in the literature³⁻⁵ and only a brief outline will be given here. A schematic illustration is given in Fig. 1. We consider a chopper with N elements which may be open or closed [$F(j) = +1$ or -1 , respectively]. The transmission of the chopper for a neutron arriving at time j is then

$$F'(j) = \frac{1}{2} [F(j) + 1]. \quad (1)$$

where the time is expressed in integral multiples of δ , the pulse width of a single element in the correlation sequence. Suppose that the chopper is phased so that the start of the correlation sequence ($j=0$) occurs at a time ℓ after the source pulse. Then the intensity recorded in a detector at time k relative to the source pulse is

$$J(\ell, k) = \sum_{i = i_{\min}}^{i_{\min} + N} F'(i - \ell) S(i, k - i) + B_k \quad (2)$$

where $S(i, j)$ is the signal recorded with a conventional chopper for incident and scattered flight times i and j , and B_k is the background at time k uncorrelated with the chopper.

We define

$$S(i, j) \equiv 0, \quad i < 1 \text{ and/or } j < 1, \quad (3)$$

and assume that, for any k , only i values within the range $(i_{\min}, i_{\min} + N)$ for some i_{\min} contribute. (The generalization to cases where this is not true is analogous to the frame-overlap situation with a conventional chopper.)

We now consider a measurement such that all values of $\ell = 1, 2, \dots, N$ are encountered with equal probability, and perform a cross-correlation on the data obtained:

$$\begin{aligned} K(i', k-i') &= \frac{1}{N} \sum_{\ell=1}^N F(i' - \ell) J(\ell, k) \\ &= \frac{1}{N} \sum_{i=i_{\min}}^{i=i_{\min}+N} \sum_{\ell=1}^N F(i' - \ell) F'(i - \ell) S(i, k-i) + \frac{1}{N} \sum_{\ell=1}^N F(i' - \ell) B_k. \end{aligned} \quad (4)$$

Let us choose a particular sequence $F(j)$ obeying these conditions:

$$\begin{aligned} \sum_{j=1}^N F(j) &= 1 \\ \sum_{j=1}^N F(j) F(k) &= (N+1) \delta_{jk-1}. \end{aligned} \quad (5)$$

Then Eq. (4) reduces to

$$K(i', k-i') = \left(\frac{N+1}{2N}\right) S(i', k-i') + \frac{1}{N} B_k. \quad (6)$$

[The restrictions of the range of i in Eq. (2) are needed because the Kronecker delta in Eq. (5) is defined modulo N .] It is seen that $K(i', k-i')$ reproduces the single-pulse scattering function but with a duty cycle $(N+1)/2N \sim 1/2$ compared with $1/N$ in the single-pulse case. The uncorrelated background only contributes with the duty-cycle $1/N$.

It can be shown the statistical gain with the correlation technique compared with the conventional technique is

$$g(i,k) \equiv \frac{[\text{rel. var. } S(i, k-1)]_{\text{conv}}}{[\text{rel. var. } S(i, k-1)]_{\text{corr}}} = \frac{S(i,k-1) + B_k}{2 \sum_i S(i, k-1)} \times M, \quad (7)$$

where M is the number of conventional measurements with the same run time that would be needed to give the required information. For example, for elastic scattering when the Debye-Waller factor is not too far from unity, we may expect $S(i,k-1) \sim \sum_i S(i,k-1) \gg B_k$ and so $g \sim M/2 \sim N/4$ if about one-half of the number of different chopper phases give useful information.

3. Experimental Configuration

The experiments were carried out at the LRMECS spectrometer with the usual Fermi chopper replaced by a correlation disk chopper of the type used in Ref. 2. [For the present measurements, however, the pattern satisfied $\sum F(j) = +1$, Eq. (5), instead of -1 as for the chopper used in Ref. 2]. The sequence of $N = 251$ elements (226 open, 225 closed) was defined by a pattern cut into a Gd_2O_3 -epoxy coating on one surface of the disk over the radius interval where the disk is illuminated by the beam; the thickness of Gd was estimated as 0.21×10^{-3} atom/cm². The transmission was measured in a separate experiment to be $<10\%$ up to about 150 meV, after which it rose rapidly to 50% at about 230 meV. In order to attenuate the fast neutron component in the beam, a single crystal of

silicon, 15 cm long x 12.5 cm diameter, was placed in the incident beam directly in front of the chopper window.

The chopper was run at a period $N\delta = 5020 \mu\text{sec}$, giving $\delta = 20 \mu\text{sec}$, which was also chosen as the channel width for the collection of time-of-flight data and the recording of the chopper phase, i.e., the indices k and l in $J(l,k)$, Eq. (2). The conditions of having all values of l occur with equal probability was satisfied simply by running the chopper asynchronously with the source. Data were recorded for total flight times corresponding to $k = 50 \dots 306$, and eight detector groups corresponding to upstream and downstream beam monitors and scattering angles of -5.7° , 14.1° , 29.7° , 63.3° , 91.5° , and 116.7° .

The LRMECS data acquisition system, with some modifications, was used for this test. This system has been previously described,⁶ so only the modifications made for this test are described here. The ordinary IPNS discriminator modules produce a 24-bit data word for each neutron event. Within this word, 20 bits contain time-of-flight information, 3 bits identify the detector input within the module, and one bit is used for status information. For the correlation chopper test, four such discriminator modules were modified so that the 20 bits which were previously used for time-of-flight information are now divided into the least significant 8 bits, which are used to represent the chopper phase relative to the accelerator t_0 pulse, and the more significant 12 bits, which are used for time-of-flight information (see Fig. 2a).

A magnetic pickup placed on the chopper generates one pulse per chopper revolution. This pulse and the accelerator t_0 pulse are fed into a CAMAC module which was built especially for the correlation chopper operation. This module digitizes the time between the last chopper pickup pulse before the accelerator t_0 pulse and the t_0 pulse itself (see Fig. 2b). This chopper phase information is digitized to 8 bits, allowing

chopper phase values from 1 to 256. This slightly exceeds the actual range of 1 to 251 used for this test. Each chopper phase value covers a span of 20 μ sec, which is determined by a scaler counting the 8-MHz time-of-flight clock signal. This 8-bit phase value is latched for use throughout the time until the next t_0 pulse, and is made available on the back of the CAMAC module.

The modified discriminator modules have connectors installed on the back so they can all be connected by ribbon cable to the 8-bit digitized phase information. The internal connections on these modules were modified to prescale the 8-MHz clock signal to provide a basic time-of-flight clock period of 2 μ sec for these modules, to shift the resulting digitized time-of-flight information to the more significant 12 bits of the 20 bits previously used for time-of-flight, and to put the 8-bit phase information appropriate to this t_0 pulse period into the least significant 8 bits in this 20-bit region (see Fig. 2a). As before, three of the remaining four bits in the 24-bit data word contains the detector address for the event and one bit contains buffer status information.

The normal IPNS histogramming software on the Z8001 microprocessor was modified to separate the 12 bits of time-of-flight and the 8 bits of chopper phase information. It then calculates the histogramming time-channel from the time-of-flight in the normal way. A maximum of 256 time-channels are allowed, and the width of these time-channels and the starting time of the first channel can be varied subject to the constraint that there is only 12-bit information available (4096 possible time-of-flight values, spanning a range of flight times from 0 to 8192 μ sec). For this particular test, all detector groups use 20- μ sec time channels. Finally, the actual channel to be incremented is calculated as

$$\text{channel} = 256 \times \text{phase} + \text{time-channel}.$$

This channel constitutes an offset within the phase-time spectrum for the detector producing the event. Events from different detectors can be grouped together, and for each such group of detectors this phase/time spectrum starts at a different location in the histogramming memory. Each such spectrum is preceded by two channels used to store the sum over the spectrum, and this sum is incremented whenever an event is histogrammed in the corresponding spectrum. With this histogramming scheme, $(256 \times 256 + 2)$ 16-bit channels are allocated in memory for each detector group. Since only 251 chopper phase values are actually possible with the chopper used in this test, some of these memory channels were never used. However, this inefficiency in the use of memory is justified by the resulting simplification in the software and in the increase in histogramming speed.

Each event is histogrammed only once, and on-the-fly time-focussing is not permitted. Aside from these minor differences and the differences in histogramming noted above, which are necessitated by the inclusion of the chopper phase as a variable, the Z8001 software is unchanged from that used by the standard IPNS systems. The run-setup software on the PDP 11-34 computer was modified to account for the allocation of channels to each detector group as noted above, and to incorporate the fact that the basic clock period used for time-of-flight in this system is 2 μ sec rather than the 0.125 μ sec used in the standard systems. Otherwise, the run-setup software is essentially the same as for normal IPNS runs. No other PDP software was changed for this test.

A run was carried out on a standard vanadium sample, 1.08 mm thick, placed at an angle of 45° to the beam in transmission geometry. Data were collected for 4.5 h before an accelerator breakdown occurred (the only major breakdown in five years of IPNS operation!) necessitating an

extended shutdown during which the correlation chopper setup had to be dismantled to make way for scheduled LRMECS experiments. It was thus not possible to carry out the planned program of an extended vanadium run followed by a background run and measurements on a series of glass and liquid samples. Nevertheless, the vanadium data obtained provide a demonstration of the feasibility of the technique.

4. Results

The vanadium data were analyzed with the usual set of programs for chopper spectrometer data analysis,⁷ modified to carry out the deconvolution of Eq. (4). As a result, data were obtained for essentially 251 different time-of-flight measurements, each corresponding to the different possible phases i' in Eqs. (4) or (6). A typical set of data, for the upstream beam monitor and the 91° detector group at $i' = 201$, is shown in Figs. 3-4. The cross-correlation procedure clearly gives the correct results for the peak positions and background.

Compared with usual results with the Fermi chopper, the peaks in both monitors and detectors appear symmetric, and the latter are centered at the calculated $E = 0$ position. Presumably this is because the chopper opening time for a single slit (20 μ sec) is symmetric and long compared with the width of the (asymmetric) source pulses at the energies used. For the 91° detector, the elastic peak from the vanadium is clearly distinguished, but there is only a hint of the much weaker inelastic scattering in the region $E = 5-20$ meV.

Figure 5 shows a plot of peak positions in the time-of-flight spectra for some of the phases analyzed. The data fall on straight lines for each monitor and the detector. The $t=0$ intercept falls at a phase $i' = -73.4, -73.2, \text{ and } -73.4$, respectively, for Monitor 1, Monitor 2, and the 91° detector, which implies that, within the accuracy of the

measurement, the pulse of neutrons leaves the source at $t=0$ for all the neutrons measured. Taking the previously measured Monitor 1-Monitor 2 and Monitor 1-sample distances of 4.755 m and 0.462 m, these values imply a source-sample distance of 6.90 m, compared with the nominal value of 6.84 m, and an effective sample-detector distance of 2.52 m compared with the expected value of 2.50 m.

The energy resolutions measured for the elastic peaks in the 91° detector were 1.5, 3.2, and 16.2 meV FWHM for $E_0 = 17.5, 25, 98$ meV respectively. This gives $\Delta E/E_0 = 9, 13, \text{ and } 17\%$ for the three energies, compared with the typical value of 8% with the Fermi choppers. This could be improved, of course, with the use of a shorter time element on the chopper. For a mechanical disk chopper, this requires a narrower slit defining the beam which considerably lowers intensities, or a higher speed of rotation. Other methods, for example, based on white-beam polarizers and spin flippers,⁸ could in principle be used also. However, even with a negligible burst time at the chopper, the resolution will at best be constant in $\Delta E/E_0$, so that ΔE will increase linearly with E . This is a serious deficiency of the method if it is used for determining the elastic structure factor in glasses, as proposed in Ref. 5.

Another possible use of the correlation technique to study the structure of fluids and disordered solids is to derive the structure factor $S(Q)$ from the area of $S(Q,E)$ at constant Q . A correlation chopper spectrometer operating on a pulsed polychromatic beam covers a substantial range of the (Q,E) plane--in fact, with considerable redundancy--and thus in principle allows the determination of $S(Q)$ in this way. This procedure, for which resolution is not as critical as for the measurement of $S(Q,0)$, avoids the kinematic corrections (the so-called Placzak corrections) which are necessary for data obtained in conventional total scattering measurements at both pulsed and steady-state sources. The

statistical efficiency of this approach has still to be evaluated, however.

In conclusion, the correlation technique at a pulsed spallation source using a mechanical pseudo-random chopper is found to be technically feasible and can be accomplished with relatively minor changes to a conventional chopper spectrometer. The strong variation of resolution with incident energy is a serious disadvantage for some applications. There may be specific instances in which the method is advantageous to the conventional chopper at such a source, but these remain to be identified.

Acknowledgment

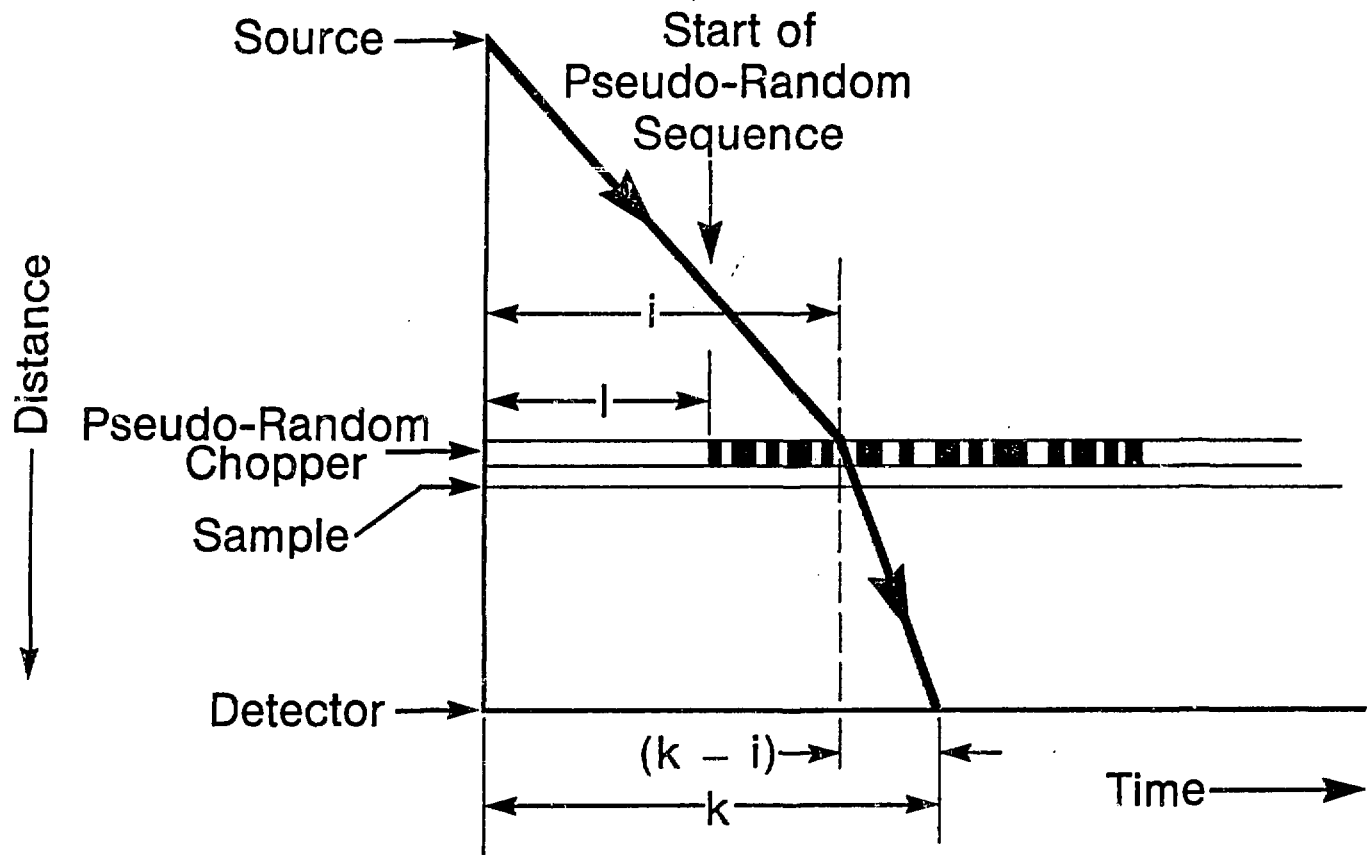
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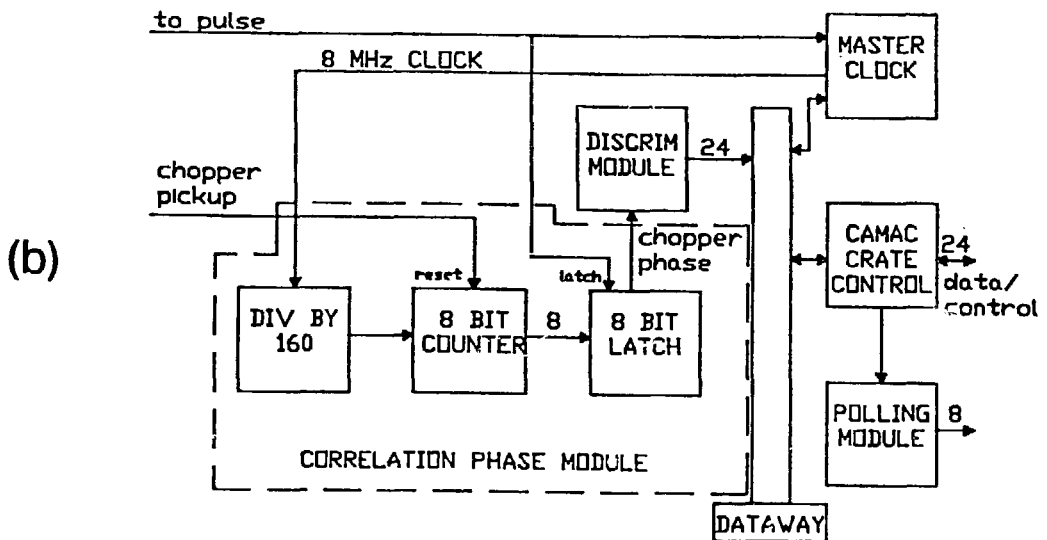
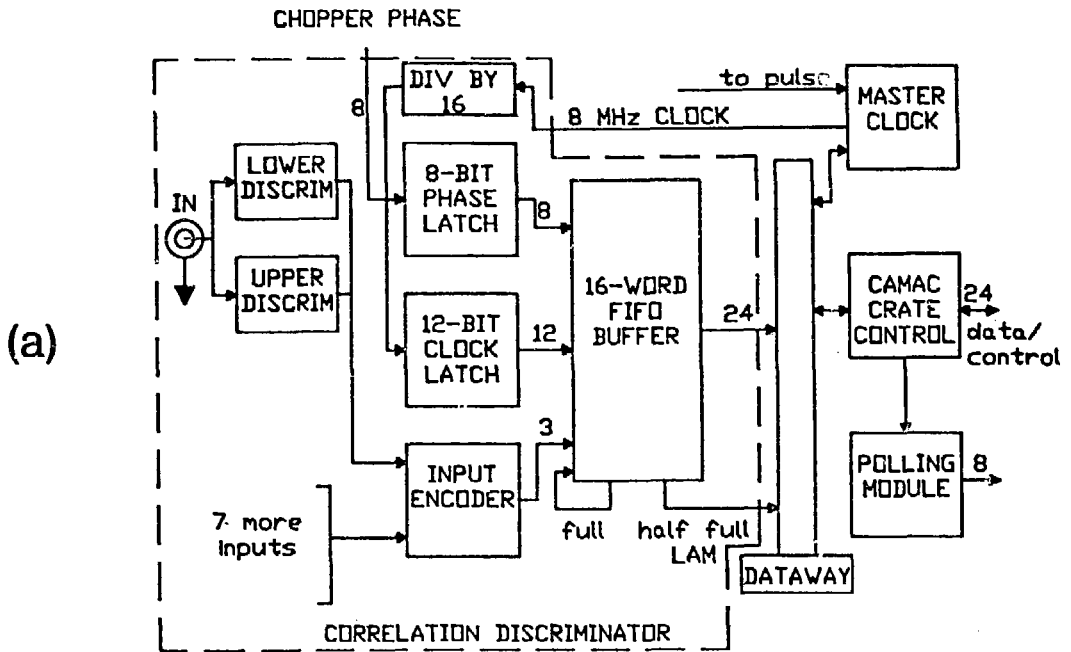
References

1. K. Sköld, Nucl. Instr. and Methods 63, 114 (1968); D. L. Price and K. Sköld, Nucl. Instr. and Methods 82, 208 (1970), and references therein.
2. K. Sköld, C. A. Pelizzari, R. Kleb, and G. E. Ostrowski, Phys. Rev. Lett. 37, 842 (1976).
3. P. Pellionicz, Nucl. Instr. & Methods 92, 125 (1971); W. Matthes, in Neutron Inelastic Scattering (I.A.E.A., Vienna, 1972), p. 773; R. Amadori and F. Hossfeld, ibid, p. 747.
4. N. Kroó, P. Pellionicz, I. Vizi, G. Zsigmond, G. Zhukov, and G. Nagy, in Neutron Inelastic Scattering (I.A.E.A., Vienna, 1972), p. 763.
5. D. F. R. Mildner and A. C. Wright, J. Non-Cryst. Solids 42, 97 (1980).
6. R. K. Crawford, R. T. Daly, J. R. Haumann, R. L. Hitterman, C. B. Morgan, G. E. Ostrowski, and T. G. Worlton. IEEE Trans. Nucl. Sci. NS-28, 3692 (1981); J. R. Haumann, R. T. Daly, T. G. Worlton, and R. K. Crawford. IEEE Trans. Nucl. Sci. NS-29, 62 (1982).
7. C.-K. Loong and D. L. Price, ANL private communication (June 1985).
8. R. Cywinski, "Polarisation Modulated Crosscorrelation Spectrometry on a Pulsed Neutron Source," Rutherford Appleton Laboratory Report NDR/P2/83 (1983), p. 36.

Figure Captions

1. Schematic diagram of the correlation technique at a pulsed source.
2. Schematic diagram of the modifications to the data acquisition electronics for the correlation chopper test. (a) Modified discriminator module; (b) new module for phase encoding.
3. Example of time-of-flight spectrum for Monitor 1 (upstream of sample), with phase $i' = 201$.
4. Same as Fig. 3 for ^3He detector at $\phi = 91.5^\circ$ (vanadium sample). The solid curve is a guide to the eye.
5. Plot of some peak positions in time for the monitors and detector versus phase used in the cross-correlation. The lines are eyeball fits through the data: they converge to $t = 0$ at $i' = 73.4$. The dashed curve (with right-angle scale) shows the values of E_0 calculated from the monitor peaks.





V, PHASE=201 CR03P201.OUT Monitor 1

Flight distance = 7.04 centroid = 2505.04 delay = 100.2

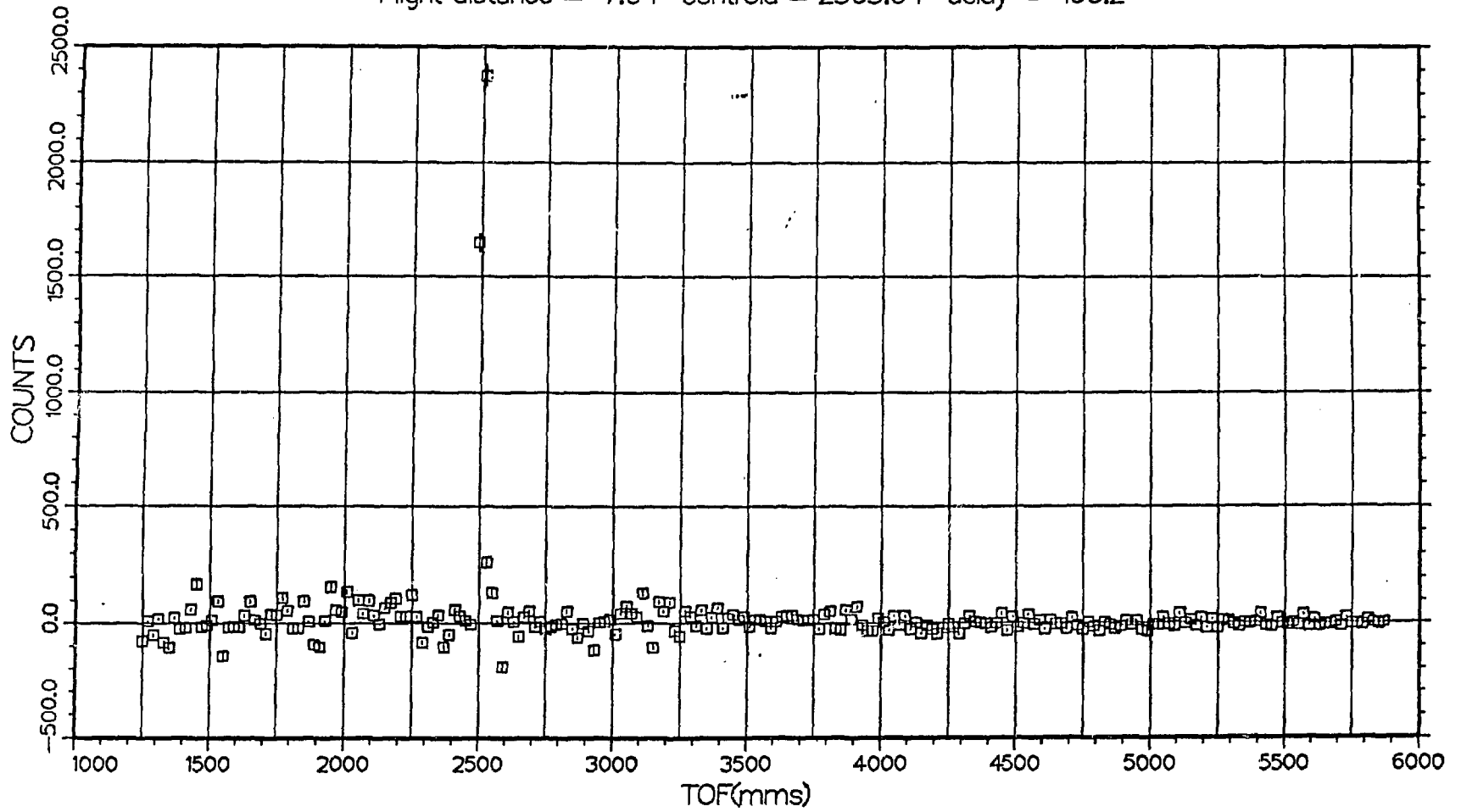


Fig 3

V, PHASE=201 CR03P201,OUT Subgroup 6 Phi= 91.50

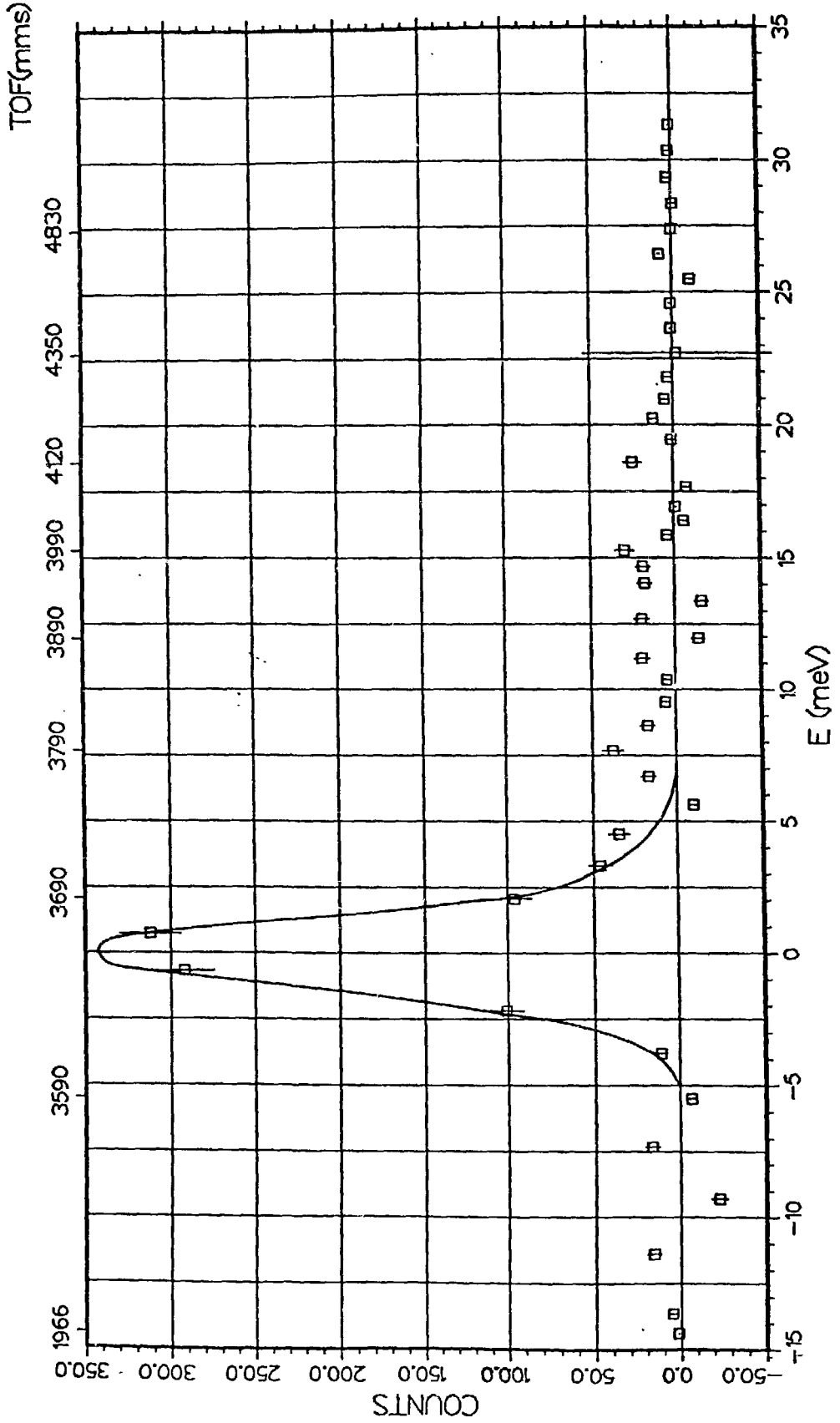


Fig 4

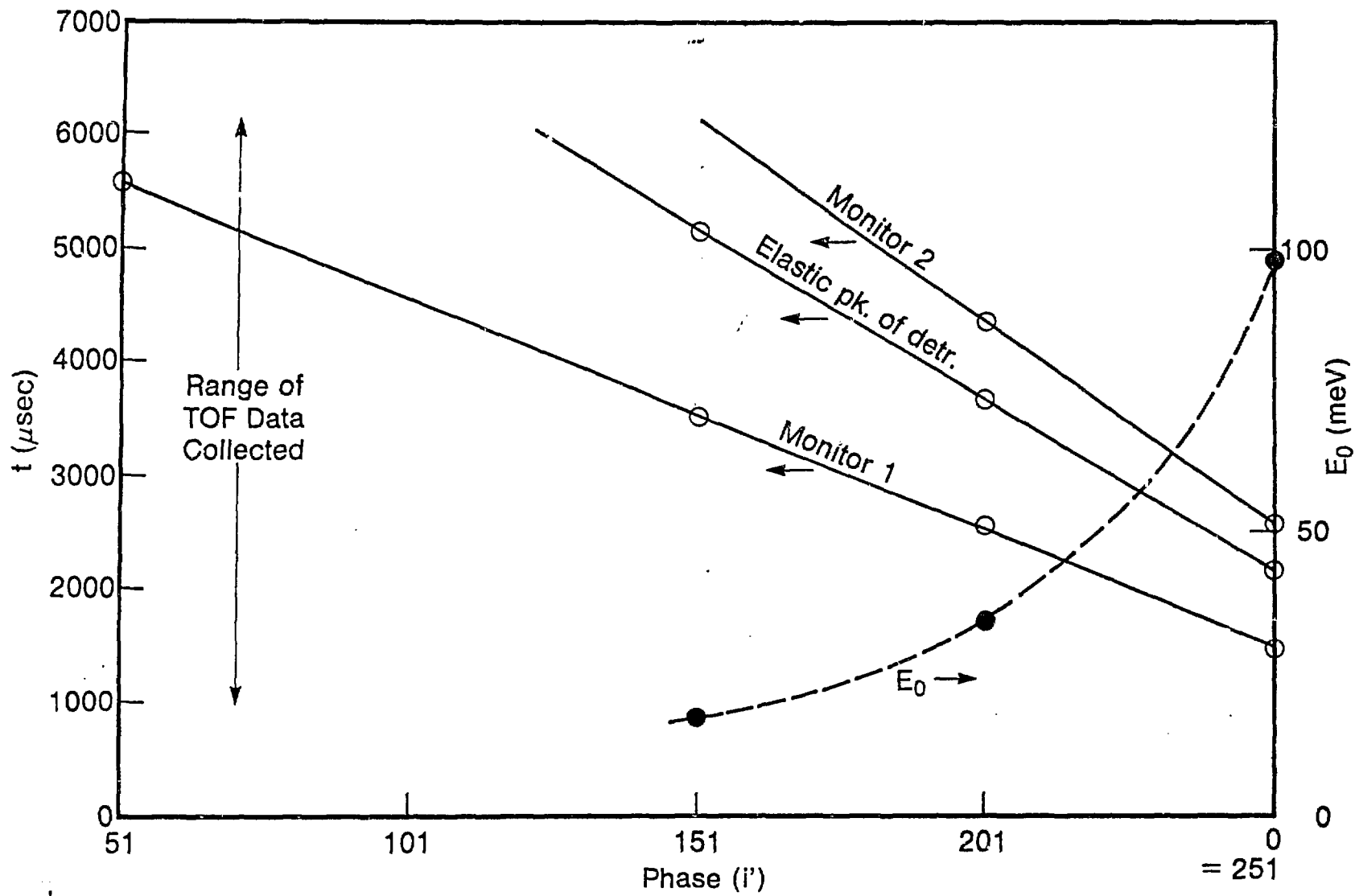


Fig 5