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*USE OF "ON LINE" COMPUTER
FOR MÖSSBAUER EXPERIMENTS*

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MINERAL SCIENCES DIVISION

Reprinted from *The Review of Scientific Instruments*,
Vol. 37, No. 3, 283-286, March, 1966

Reprint Series RS 46



1867 | 1967

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ROGER DUHAMEL, F.R.S.C.

Queen's Printer and Controller of Stationery

Ottawa, Canada

1967

Use of "On Line" Computer for Mössbauer Experiments

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(Received 19 May 1965; and in final form, 17 November 1965)

The application of a small general purpose computer as an "on line" data acquisition device for Mössbauer effect experiments is described. A method of conversion from analog to digital information and an outline of the computer program are given. The performance of the system is demonstrated by a Mössbauer spectrum of iron sulphide (pyrite). The extension of these techniques to other experiments is briefly considered.

INTRODUCTION

THE use of a small, general purpose digital computer for complex nuclear physics experiments has been widely described in recent literature.¹⁻³ Most of these experiments involve multiparameter pulse height analysis, and the computer has been generally used as a data acquisition device and control element rather than a data processor. Such systems are a logical extension of the multi-channel analyzers which have been commonly used for many years in nuclear physics research. It is felt, however, that there are many other experiments which can successfully employ an "on line" computer for data acquisition.

In the use of a computer as an "on line" data acquisition device, four different aspects must be considered, the conversion of the analog input signals to binary numbers, the interfacing of the converter to the computer, the program sequence of the computer, and the control of the experiment by the computer.

INPUT CONVERSION

The system used for the Mössbauer effect experiments is shown in Fig. 1. All the elements, with the exception of the continuous analog-to-digital converter (CADC) are standard devices and have been described in the literature.⁴ The input to the CADC is a signal derived from the velocity transducer, and the converter output is a set of binary numbers proportional to this input signal. The general method of the conversion process is shown in Fig. 2. The comparator circuit compares the input voltage to the voltage from the digital-to-analog (DA) converter and operates the control circuit. When the input signal is greater than the DA signal, the counter counts up; the counter counts down when the reverse is true. The number in the counter is therefore representative of the value of the input signal.

There are two parameters commonly used to describe the performance of an analog-to-digital converter. The equation describing the operation of a converter is $V = kN$, where V is the input voltage, k is a constant, and N is the channel number. The integral linearity is defined as $\bar{k}_0 - \bar{k}_{\max}/k$, where \bar{k}_0 is the average value of k over the first twenty channels and \bar{k}_{\max} is the average value of k over the upper twenty channels. Thus the integral linearity

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¹ *Proceedings of the Conference on the Utilization of Multi-Parameter Analyzers* (Columbia University, New York, 1962), Rept. No. NYO 10595.

² H. L. Davis, *Nucleonics* 22, No. 12, 47 (1964).

³ J. F. Whalen, J. W. Meadow, and R. N. Larsen, *Rev. Sci. Instr.* 35, 682 (1964).

⁴ R. L. Cohen, P. G. McMullen, and G. K. Wertheim, *Rev. Sci. Instr.* 34, 671 (1963).

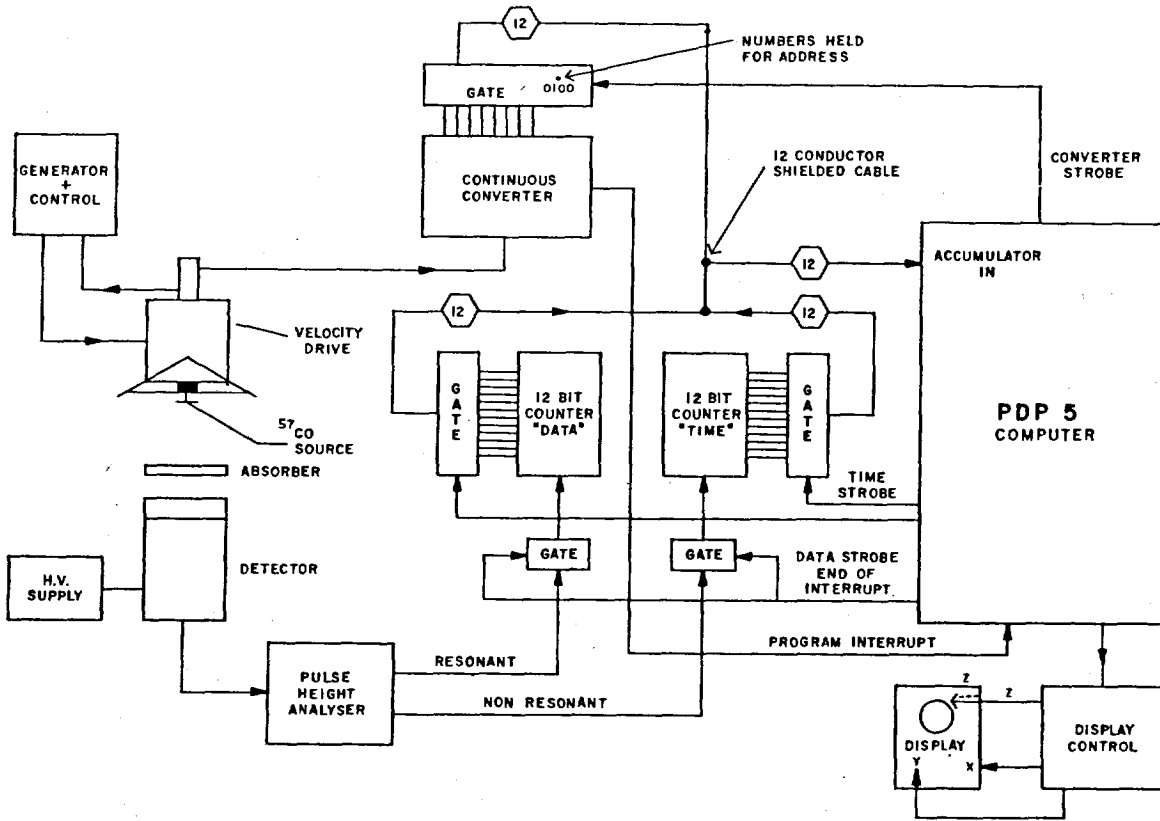


FIG. 1. Block diagram of experiment using "on line" computer.

describes the deviation of the actual performance of the converter from a linear conversion of voltage to channel number. The differential linearity is defined as the maximum deviation of k from an average value and hence describes the variation in effective channel width. Thus the differential linearity symbolically is $\Delta k/\bar{k}$, where Δk is the deviation and \bar{k} is the average value. The converter used for these experiments encoded twelve bits of which the eight most significant bits (MSB) were read as a channel

address. The comparator circuit was sensitive to $\frac{1}{2}$ least significant bit (LSB) and thus the average deviation of channel width, assuming a continuum of input amplitude, is $\frac{1}{4}$ LSB. Thus, differential linearity of this system is one part in 2^8 or 1.5%. The integral linearity has been measured to be better than 0.5%. These parameters were measured for low frequency waveforms where the converter could follow the changes in input waveshape. The converter clock operates at a 1 Mc rate and for the 12 bit system the

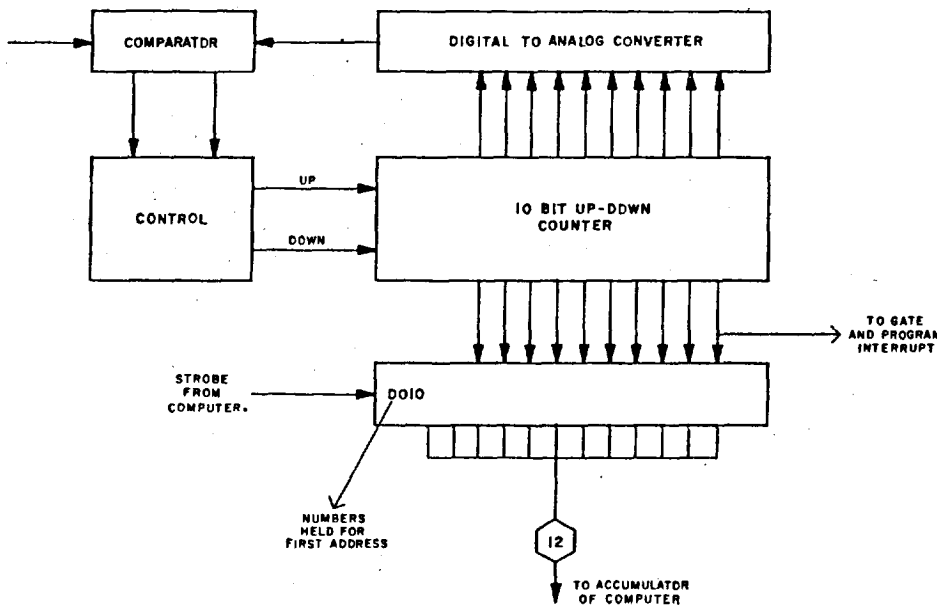


FIG. 2. Continuous analog-to-digital converter block diagram.

converter could follow changes in waveform that occurred more slowly than 1 msec. For the low frequency (8 cps) waveforms used in Mössbauer experiments the converter followed the input waveshape with no difficulty.

As mentioned previously, the converter used in this system is a 12 bit device of which the 8 MSB are read and used as an effective address for the system. Hence the last four bits may oscillate and not affect the accuracy of the converter or generate false information into the computer. A change in the 8th bit generates a pulse which stops the "data" and "time" counters and generates a "data ready" signal pulse for the computer. These two counters accept input information from the resonant and nonresonant channels of the single channel analyzers and are used as temporary storage for input data. It is only when a whole channel has been changed in the velocity spectrum that these counters are stopped and read. The counting rate of these counters is 2 Mc which is much faster than the detecting system in use for the Mössbauer experiments. The total time of transfer is 24 μ sec for both counters, and for an 8 cps waveform the average time between transfers is 500 μ sec. A buffered storage system is used so that the experiment may be restarted within 1 μ sec after the channel advance has been initiated.

INTERFACE

The output of the CADC and the two 12 bit binary counters are coupled to the computer through the gates, as shown in Fig. 2. When these gates are opened upon command from the computer, the information from the buffers of the CADC and the two 12 bit counters are transferred to temporary storage locations in the computer. Since the CADC, counters, and computer are made from the same type of circuit modules, there is no problem with voltage levels or pulse widths when interconnecting the various units.

PROGRAM

The computer used for these experiments is a Digital Equipment PDP-5.⁵ This machine has a 12 bit binary word length and a storage capacity of 4096 (2^{12}) words. It is equipped with a "program interrupt" facility which allows an external device to temporarily interrupt a program and start another. This second program, called the "interrupt service routine," is generally short and is designed exclusively to service the device which generates the interrupt. At the end of this service routine, the computer transfers back to the main program and resumes at the point at which it was interrupted. For these experiments, the main program continuously displays the con-

tents of the "data" or "time" register on the computer controlled oscilloscope. The choice of information to be displayed is selected from the input teletypewriter.

When the CADC generates a "data ready" pulse, the program interrupt is initiated. The interrupt service routine reads the contents of the "data" and "time" counters and the CADC from their buffer registers and transfers the binary information to a temporary storage location in the computer memory. It then clears the buffer registers and proceeds to process the information temporarily stored. This entire sequence takes 192 μ sec. The contents of the CADC, now in temporary storage, are used as an address (often referred to as a "channel number" in conventional pulse height analyzers). To the contents of this address (or channel) are added the contents of the register temporarily storing "data." The contents of the register temporarily storing "time" are added to a corresponding area in another part of memory. Two registers are used for each data point since the capacity of one register is only 4096 (2^{12}) counts. By using one register to count the overflow of another, the maximum number of counts is increased to 16 777 216 (2^{24}) counts.

In addition to the live display of the experimental results, the computer was programmed to calculate the ratio of the "data" and "time." Output programs stored in the computer were used to type out the contents of the two registers or the ratio of these. The output procedures are initiated by typing the appropriate command character on the input teletypewriter. In addition, the computer upon request produces a punched paper tape containing the experimental results. This tape may be fed into a large central data processing system for further processing and analysis.

EXPERIMENTAL RESULTS

A typical Mössbauer spectrum of iron pyrite is shown in Fig. 3. This spectrum has been plotted directly from the computer output with all corrections for normalization and solid angle having been performed by the computer. This spectrum shows the Mössbauer effect in three orientations of a large single crystal of iron pyrite and indicates that the principal electric field gradient axis lies along the [111] direction.

COMPARISON OF USE OF "ON LINE" COMPUTER WITH CONVENTIONAL MULTI-CHANNEL ANALYZER

Because of the simplicity of the experimental procedures involved in obtaining Mössbauer effect spectra, the use of a computer would seem an unnecessary complication. However, for Mössbauer experiments most workers use multichannel analyzers which are of similar complexity. The chief advantage of the computer lies in its versatility;

⁵ Digital Equipment of Canada Limited, Carleton Place, Ontario, Canada.

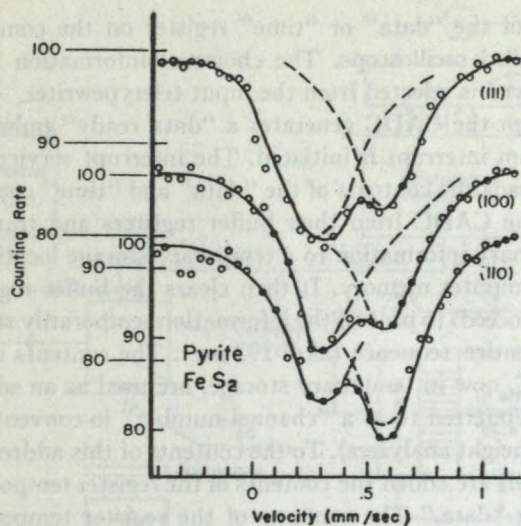


FIG. 3. Mössbauer spectrum of oriented pyrite.
Velocity scale from iron.

the computer can be used as a data acquisition device for many types of experiments and, if memory is sufficient, these experiments may be run simultaneously. The only requirement for such experiments is that the desired parameters can be converted into binary numbers (using, for example, a CADC), and the input information changes at a rate of not greater than approximately ten thousand times per second (10 kc).

The commonly used method of Mössbauer spectroscopy used a multichannel analyzer operating in a time mode. In this mode, the channels are advanced at a given fixed rate and the number of counts per channel thus represents a time spectrum. If a constant acceleration velocity drive is used, this time spectrum corresponds to a velocity spectrum. There are several problems with the technique involving the determination of the position of zero velocity and the synchronization of the time and velocity sweep circuits. In the system used with the computer the velocity is actually measured rather than assumed to vary linearly with time, and thus small deviations from linearity of

the drive become unimportant. No synchronization or zero velocity problems exist. There is a constant deadtime with the computer of 0.25% whereas the deadtime with a typical multichannel analyzer is in the order of 20–30%. This improvement in the amount of deadtime, in general, only decreases experimental time when long lived isotopes are used and data accumulation rates are not high. The continuous analog-to-digital converter could be eliminated and the computer also operated in a time mode, but it is felt that this is not as satisfactory a system as the actual measurement of the velocity. For short lived or Coulomb excitation this decrease in deadtime is more important.

The other advantage of a computer is that it is capable of performing division, and thus by using resonant and non-resonant portions of the gamma-ray spectrum, an automatic correction for solid angle changes may be made. This ratio may be displayed on the oscilloscope. The resultant display gives a truer picture of the actual Mössbauer effect spectrum under study than displaying the raw data. In many situations, the computer can be used to control an experiment and, in doing so, greatly simplify data acquisition. In the present experiments, the computer was used to control the reading of the various counters but was not used to control the progress of the experiment. If, however, a spectrum as a function of temperature, magnetic field, pressure, or some other parameter were desired, the computer could be programed to control this parameter and perform a series of data accumulations for various predetermined values. Further experiments of this nature are being planned.

ACKNOWLEDGMENTS

The authors wish to thank D. J. Doyle, J. Mutzeneck, and W. MacGregor of Digital Equipment of Canada Limited for their help in this work. C. A. Josling and A. H. Bettens of the Department of Mines and Technical Surveys aided in the running of the experiments, and their assistance is appreciated.