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A MÖSSBAUER-EFFECT DATA-COLLECTION SYSTEM

by

R. H. Vonderohe and
R. A. Aschenbrenner

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Applied Mathematics Division

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November 1967

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INTRODUCTION

This report describes the general system configuration and utilization of a small, general-purpose digital computer used for data acquisition from, and minor control of, four Mössbauer-effect experiments.

The Mössbauer effect is an example of nuclear-resonance fluorescence in which the nuclear gamma rays are extremely sharp. This sharpness derives from transitions in which the lattice does not change its energy state when the gamma ray is emitted. Because of the sharpness, the resonance can be scanned through Doppler-shifting of the gamma-ray energy by moving a source with respect to a scatterer, or, more usually, an absorber. There is then a marked change in the nuclear scattering or absorption as the relative velocity is varied. The spectrum of counting rate versus velocity may be used to study hyperfine structure of the nuclear states. The final state of the gamma-ray transition is always the ground state of a nucleus sufficiently stable to be available in the quantities needed for an absorber or scatterer. This state may be studied by other means, but the Mössbauer effect is a powerful tool for the study of low-lying excited states of nuclei. Also, and possibly more importantly, when the properties of the states are known, the Mössbauer effect can then be used to study the atomic properties which in part produced the hyperfine interaction. In this way, it becomes a tool for solid-state physics and for chemistry.

Various types of velocity spectrometers are used in Mössbauer-effect measurements. The velocity ranges are generally less than 10 cm/sec and can be as small as a few microns/sec. The following procedure is frequently used in obtaining the energy spectrum: The absorber is placed on a piston drive or similar mechanism. A shaft, attached to the piston, is connected to a rotating flywheel, which drives the absorber toward and away from the source as it rotates. Figure 1 is a sketch of a typical drive mechanism. Each half-cycle is typically divided into 200 equal time periods, during each of which the number of detector pulses is counted.

At the limit of each half-cycle a free-running oscillator is started. This oscillator is resynchronized each half-cycle. The oscillator pulses, called channel-advance pulses, indicate when the accumulated detector

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Fig. 1. Typical Mössbauer-effect Drive Mechanism

pulses are to be stored. Typically this storage has been accomplished in a "time" or multiscaler mode analyzer. Since the energy spectrum resulting from absorber motion toward the source is different from the spectrum for motion away from the source, the channels are stored individually. This procedure then requires a 400-channel analyzer.

Each experiment will typically complete approximately three cycles per second, although some experimental devices are used at faster or slower rates. This frequency results in 1200 channels per second. The number of counts per channel varies significantly from several counts to possibly several thousand.

With the above-mentioned principles and data rates in mind, coupled with the decreasing price of general-purpose digital computers, the system about to be described was assembled at Argonne. This device is for use with four velocity spectrometers, which derive their motion from a mechanical device rather than an electromagnetic transducer. It replaces four pulse-height analyzers operated in the "time" or multiscaler mode.

GENERAL DESCRIPTION

A prime consideration in selecting a general-purpose digital computer for this application was the time required for information storage. This consideration was closely related to another prime consideration, the number of bits

required for the storage of a single channel, both on an incremental basis and on a total-accumulation basis.

With regard to the first consideration, the four experiments were capable of supplying 4800 channels per second. Therefore, the computer had to be able to accept channels on the average of every $208 \mu\text{sec}$. This requirement was not particularly stringent. Regarding the second consideration, with an incremental storage requirement of several thousand counts, a 12-bit input facility was determined to be sufficient. However, the total accumulation per channel required that 24 bits be allocated.

An additional requirement placed on the computer was that of a display capability. Each analyzer used previously was capable of displaying the accumulated channels that were stored within it. Obviously the computer had to provide a similar capability.

After due consideration, not the least factor of which was cost, the Scientific Control Corporation 650 computer was selected. (Figure 2 is a photograph of the SCC-650 computer.) This small, general-purpose digital

145-997

Fig. 2. SCC-650 Computer with Typewriter

computer has a 12-bit word length and 4096 words of core memory with a memory cycle time of 2 μ sec. The machine has hardware memory protect, accumulator, hardware index register, and numerous micro-programmable instructions, in addition to normal arithmetic, literal, and input-output instructions. Input-output may be accomplished either through the accumulator or through the Direct Memory Access (DMA) Channel, which shares the memory with the Central Processing Unit (CPU) on a cycle-steal basis.

In addition to the computer mainframe, the manufacturer supplied a Tektronix 503 rack-mounted oscilloscope. This oscilloscope was interfaced to the computer through two 10-bit digital-to-analog converters, which are set by the lower-order 10 bits of the accumulator. One converter generates the X deflection voltage, and the other the Y deflection voltage. The facility for incrementing either the X or Y deflection by one position is also provided with the appropriate command. The following oscilloscope commands are provided:

- Load X
- Load Y
- Increment X
- Increment Y
- Load X and Intensify
- Load Y and Intensify
- Increment X and Intensify
- Increment Y and Intensify
- Intensify Only

Only the Load X or Load Y commands refer to the accumulator. The utilization of these commands will be discussed in the section on the control program.

The standard input-output device associated with this computer, and with many others, is the Teletype ASR-33. This unit combines the features of a keyboard, printer, paper-tape punch, and paper-tape reader. These functions are normally operated by the central processor through the accumulator at an operating speed of 10 characters per second. In addition, the unit may be operated off-line for paper-tape preparation or duplication.

EXPERIMENTAL INTERFACE

The most efficient means available to input data is the Direct Memory Access (DMA) feature. This feature permits information to be stored into or extracted from memory without the execution of an instruction by the Central Processing Unit (CPU). The use of this feature permits the CPU to perform the data manipulation required for the display function and to perform the other necessary control and output functions.

To use the DMA, the memory must be supplied with address lines to indicate the memory location to be used--either for storing or extracting information. There are 12 of these address lines; used in parallel, they permit the utilization of any of the 4096 available memory locations. Additional lines that must be supplied are as follows:

12 Data Lines In
 12 Data Lines Out
 1 Read/Write Control Line
 1 DMA Request Line
 8 Timing Lines

Figure 3 shows a typical DMA interface.

However, the interface necessary for four experiments required more than the standard interface. In addition, it was desirable to accomplish the double-precision (24-bit) channel storage without program intervention. Toward this end, a special experimental interface was constructed. Figure 4 is a block diagram of this interface. Although only one experiment is shown in detail, each of the other three operates in the same manner.

Fig. 3. Standard DMA Interface Representation

Each experiment supplies four different signals to the interface. The Zero Reset and 200 Reset signals are supplied by photoelectric detectors associated with the rotating flywheel. At the beginning of each half-cycle of rotation, one of the two reset signals is generated by means of a slot in the flywheel. External to the interface, the reset signals are used to resynchronize the free-running oscillator.

The signals from the detector, corresponding to the unabsorbed gamma rays, are fed directly to a 12-bit binary counter. When a free-running oscillator pulse is received, signifying channel advance, the state of the 12-bit binary counter is transferred to a 12-bit buffer. This transfer is accomplished in approximately 1 μ sec, which is then the experiment dead time.

The channel-advance pulse is also fed to the main interface control. Upon receipt of the channel-advance pulse, and assuming that another experiment is not in the process of storing a channel, the control unit initiates

a "read" memory cycle. The memory location that is read is indicated by the address counter associated with the experiment. The word read out will be the lower-order 12 bits of the current channel. These 12 bits are then added to the 12-bit buffer in the 13-bit adder. The total is then stored back into memory in the same location via a write cycle.

Fig 4. Special DMA Interface, Block Diagram

When the information has been stored, the 13th bit of the adder is checked by the control unit. If this bit is a 0, the address counter is advanced by two and the main control awaits the next channel-advance pulse. If, however, the 13th adder bit has the value 1, signifying an overflow, the address counter is advanced only by one. A "read" is then initiated, and the most significant 12 bits of the channel are read out to the adder. When the read has been performed, 1 is added and the new word is then stored back into memory. The address register is then advanced by 1 again, and the next channel-advance pulse is awaited. This procedure results in successive channels being stored in successive pairs of memory locations.

In addition to resynchronizing the free-running oscillator, the "reset" signals perform another function. Associated with each experiment, on the front of the interface, are three rows of toggle switches--two rows of twelve and one row of six. (Figure 5 is a photograph of the interface panel.) The experimenter sets these rows of switches before initiating the experiment. The two rows of twelve switches each are set as binary addresses for channel storage in the computer memory. The first row of switches indicates the starting address for the first half-cycle of the experiment. The second row indicates the starting address for the second half-cycle of the experiment.

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Fig. 5. Mössbauer Experiments--Computer Interface Panel

A Zero Reset signal will force the address counter to the state given by the first row of switches, and a 200 Reset signal will force the counter to the state of the second row of switches. The third row of switches is used for experiment protection. The six switches in this row correspond to the most significant 6 bits of a 12-bit address. The state of this row of switches is used as an upper limit for channel storage for the experiment. This precludes a malfunction of one experiment from destroying information from another experiment.

A typical experiment would proceed as follows: First the experiment would be initiated by a Zero Reset signal, which would set the address and synchronize the free-running oscillator. Detector pulses would be counted by the 12-bit counter until a channel-advance pulse was received. The channel-advance pulse would cause the accumulation in the counter to be transferred to the buffer. Following the transfer, the counter would be cleared. Then the counter would start counting detector pulses for the next channel. The control unit would then initiate the read cycle, and the add

would be performed. Once the sum had been stored back into memory, the overflow checked, and the address counter incremented appropriately, the next channel-advance pulse would be awaited.

This process would continue until the 200 Reset signal was received. By a judicious choice of oscillator crystals, the 200 Reset signal is always received before accumulating the 200th channel. This precludes double storage in the channels from number 200 and up. Upon receipt of the 200 Reset signal, the address for channel 200 is set into the address counter. The same channel-advance procedure is now followed until the Zero Reset signal is again received.

The usual situation is collection of data from more than one experiment at any given time. When this is the case, the experiments are serviced on a cyclic request basis. Sufficient time is available to accommodate all four experiments if they should issue channel-advance pulses simultaneously.

In addition to the normal accumulation functions of the interface, facilities are provided for testing each experiment and for clearing any or all of the section of core memory associated with each experiment. The interface utilizing the DMA feature may operate irrespective of the running program and will even operate if the CPU is in a halt condition.

CONTROL PROGRAM

The hardware necessary for data acquisition having been provided, it remained to provide a program that would communicate with the experimenter and perform certain desirable tasks. Therefore, a program called Möss. Control was written for this purpose. The experimenter can communicate with the program via the teletype keyboard using coded instructions.

The initial function of the program is to set up and arm the interrupt system. Once the system is armed, the experimenter may gain control by striking any teletype key. When an interrupt occurs, the interrupt system is disarmed, and the teletype prints OK and then waits for a coded instruction. To conserve memory space, these coded instructions were kept as short as possible.

There are eight possible coded instructions for control of the experiments:

S1, S2, S3, S4
H1, H2, H3, H4

These instructions "Start" or "Halt" the four experiments (e.g., S1 = Start Experiment No. 1). As previously stated, the experiments may enter data

into memory, even when the CPU is in a "Halt" condition. A MEMORY START-STOP switch is provided on the interface panel for each experiment. When this switch is in the STOP position, the program may override the switch to start or stop the experiments as instructed. This is the normal mode of operation. Upon execution of the start or stop command, the program recovers from the interrupt by rearming the interrupt system and returning to the instruction stream that was being executed before the interrupt.

One of the more important functions of the control program is that of displaying the accumulated channels from the various experiments. When the experimenter types DS, following the initiated interrupt, the control program enters the display routine. The first action by the display program is to request the starting address of the channels to be displayed. This is done by typing out SA on the teletype. The experimenter then types four octal digits, which are the location in memory of the first channel to be displayed. These four digits may be read directly from the interface switches for the particular experiment if channel Zero is the first one desired. If other than channel Zero is desired for the first channel, the address indicated by the interface switches must be modified.

When the four octal digits have been typed in, the starting location is stored and the program then requests the number of channels to be displayed. This is done by typing out NC on the teletype. The experimenter now types three decimal digits, which are stored by the program. Following the storage of the number of channels, the program requests the scale factor for display by typing out SF on the teletype.

As previously stated, each channel is stored in two successive memory locations, which allows 2^{24} counts. Since the display is limited to 2^{10} accuracy, it is necessary to select the ten bits to be displayed. This is the reason for the scale factor. Each channel is viewed as a 24-bit number. There are 15 possible scale factors associated with these 24 bits, ranging from the least significant 10 bits to the most significant 10 bits.

When SF has been typed out by the program, the experimenter responds by typing two decimal digits. These digits may range from 00 to 14, corresponding to the 15 different scale factors. If the two digits typed are not within this range, an error indication is given and a correct scale factor is requested. If the experimenter types a legitimate scale factor, the program immediately begins displaying the requested channels. This actual display portion of the routine is a continuous loop, which displays the channels dynamically; that is, the total accumulations may be seen to be changing.

The display routine also performs another function with regard to the number of channels to be displayed. Since the digital-to-analog converter

provides 1000 points in the X direction, it was deemed desirable to incorporate an automatic X scale factor based on the number of channels to be displayed. It would then appear to the experimenter that the gain was a function of the number of channels. This feature was accomplished in the control program by varying the horizontal space between points, based on the number of points. Break points were established as follows: If the number of channels is at least 500, the space between points is 1; if the number of channels is 330 or greater but less than 500, the space between points is 2; between 250 and 330, the space is 3; etc. Table I summarizes breakpoints versus point spacing. (Figure 6 is a photograph of an actual display showing accumulated channels with absorption peak.)

TABLE I. Display-point Spacing

No. of Channels	Space between Points	No. of Channels	Space between Points
500-1000	1	100-199	5
330-499	2	50-99	10
250-329	3	<50	20
200-249	4		

Once the display has been initiated, the program rearms the interrupt system. If the experimenter desires to start or halt any of the experiments or alter any of the display parameters, he may then do so. If he desires to halt the display, an interrupt followed by an SD type-in accomplishes this. The interrupt system is then armed again. When a display is being performed and the experimenter causes an interrupt to alter the status of an experiment, the display is temporarily halted. Upon completion of the desired function, the display resumes.

The one remaining function of the control program is that of outputting the accumulated data. The coded command TC (type channels) has been designated for this purpose. Following an interrupt, the characters TC, when typed on the keyboard, cause the program to enter the output routine. The program then types out EXP. ST. ADD. and waits. The experimenter then types four octal digits, which correspond directly to the switch register on the interface panel for the experiment. In this case, the octal address is not modified. This type-in is followed by the type-out ST. CH. NO. (starting channel number). For output, the contents of each channel are preceded by the channel number relative to the experiment. The first channel output may be anywhere within the experiment. The experimenter must type in three decimal digits for the starting channel number. Following this type-in, the program responds by typing out NO. of CH. (number of channels). This typeout is answered by three decimal digits indicating the number of channels to be output.

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Fig. 6. Experiment Display

At this point the program comes to a halt. The experimenter now has the option to accept either a type-out alone or a type-out with a paper-tape punch-out. If a type-out alone is desired, the experimenter restarts the computer and the requested number of channels are typed out with channel numbers. This type-out prints five channels per line. (See appendix.)

When the experimenter desires a punch-out as well as type-out, he turns the punch on while the computer is halted. At this time, paper-tape leader is run out and any desired preliminary information such as date, run, number, etc., may be punched by merely typing. When the preliminary information has been entered, the experimenter restarts the computer and the desired channels are punched as well as typed. When the type-out or type-punch-out has been completed, the computer again halts. At this time, tail-type paper tape may be run out, the punch turned off, and the paper tape removed for data processing. Restarting the computer then causes recovery from the original interrupt and a return to the original instruction stream.

During this output routine, the program must perform numerous tasks. In the category of bookkeeping, the number of channels as well as the channel number must be monitored and modified as required. Since the channels are stored individually as double-precision binary quantities, the program must perform a 24-bit binary-to-decimal conversion for each channel requested. This conversion is accomplished by using an excess-three procedure with bin-type binary-coded-decimal temporary storage. The result of the procedure is a nine-decimal-digit quantity for channel content.

Selection of the excess-three method of binary-to decimal conversion was based primarily on the fact that the method was iterative in nature, thus conserving limited memory space. At present, the control program occupies approximately 1000 memory locations, or one-quarter of the total available. Table II summarizes the available responses to an interrupt.

TABLE II. Response Commands to an Interrupt

S_1 = Start Experiment No. 1	S_4 = Start Experiment No. 4
H_1 = Halt Experiment No. 1	H_4 = Halt Experiment No. 4
S_2 = Start Experiment No. 2	DS = Start Display Routine
H_2 = Halt Experiment No. 2	SD = Stop Display Routine
S_3 = Start Experiment No. 3	TC = Punch and/or Type Channels
H_3 = Halt Experiment No. 3	

CONCLUSIONS

The system described here has several advantages over running the same number of experiments, each with a dedicated analyzer. First, the cost of the computer system is approximately 30% less than the cost of four analyzers. In spite of this price differential, there is no loss of versatility to the experimenter (assuming, of course, there is no catastrophic failure). In fact, the computer system offers a great deal more versatility, particularly in the area of data preprocessing.

It is now possible to do such things as channel summations, spectra folding, and exact peak center determinations, which were previously unrealizable with analyzers. In addition, energy calculations that previously required additional computing power may now be performed. Another advantage of this system is the capability of outputting an experiment and reloading the same experiment at a later time for additional data storage. In short, the system has all the advantages of a general-purpose digital computer in addition to performing the tasks of a wired-program analyzer.

APPENDIX

Sample Printer-Keyboard Sequences

The actual printer-keyboard sequence, with errors, for starting Experiment No. 1 and displaying accumulating data is as follows:

OK		3000	
SQ	ERROR	NC	
OK		400	
S1		SF	
OK		16	ERROR
DS		SF	
SA		06	

This sequence indicates the computer-experimenter response for the initiation of Experiment No. 1 and the display of 400 channels starting at memory location 3000 at a scale factor of 6. (The bottom of the display will correspond to 64 or fewer counts.)

The actual printer-keyboard sequence for halting Experiment No. 1 and typing channels 10 through 19 of this experiment are as follows:

OK	3000
H1	ST. CH. NO.
OK	010
TC	NO. OF. CH.
EXP. ST. ADD.	025

```
010 000156784 011 000157072 012 000158277 013 000157656 014 000157629
015 000156545 016 000157114 017 000156832 018 000158224 019 000157618
020 000157442 021 000158181 022 000156967 023 000157457 024 000157492
025 000157366 026 000158592 027 000156009 028 000157659 029 000157630
030 000157185 031 000157256 032 000157139 033 000157947 034 000157108
```

This sequence indicates the computer-experimenter response for halting Experiment No. 1 and the type-out of the accumulated counts for 25 channels starting with channel 10. The peak is seen to be at channel 27. Channel 0 is located at memory location 3000. The control program provides halts after the type-in of the number of channels and after completion of the type-out to enable the experimenter to turn the punch on and off if paper tape is also desired.

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