COMPUTER CONTROL OF A MULTICHANNEL SCALER AND QUADRUPOLE MASS FILTER WITH AN IBM PC

T. S. YEH (葉泰聖) AND T.-M. SU (蘇志明)

Department of Chemistry, National Taiwan University, Taipei, Taiwan 107, R.O.C.

H. C. LIN (林許成)

Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan 107, R.O.C.

Key Word Index—Microcomputer interface; multichannel scaler; quadrupole mass filter; microcomputer.

An interface for a Canberra Model 7880 fast multiscaler and an Extranuclear quadrupole controller with an IBM PC is described. With the interface and using only a few keystrokes one can choose to take either a mass spectrum or a time-of-flight spectrum of a given mass. The limitations and the minor modifications of the original hardware are also discussed.

Electron multipliers and channeltron electron multipliers are widely used as thermal energy particle detectors. One can easily encounter either one of them in a commercially available mass spectrometer. For UV-VIS photon detection, such as is necessary in a fluorometer, a photomultiplier tube is freqently used. Depending on the follow-up electronic systems, both types of the detectors can be used in either digital mode or analog mode.

When detecting low photon signals or low particle signals, which frequently occur when measuring the luminescence decay time of molecules or the time-of-flight (TOF) spectrum of photodissociating fragments, the digital mode is generally regarded to be superior. One of the reasons is that the digital method can eliminate the dc leakage component of the dark current and also the dark current components originating from secondary electron emission from the surface[1]. A further reason is that the digital data can be processed easily by a microcomputer.

The control center of the digital method is usually a multichannel analyser capable of multichannel scaling and pulse height analysis. Manufacturers have also frequently offered a wide variety of delicated modules for specific functions, such as fast multichannel scalers or fast analog-to-digital converters, that could match their own multichannel analysers. Commercial multichannel analyser systems are usually self-contained and free of trouble. However, they sometimes suffer from several drawbacks: their system structures are not very flexible and many of the built-in functions may never be used and are not necessary for the specific task. Finally the question of financial affordability often needs to be addressed.

In this paper we report the use of an IBM PC, a widely available general purpose microcomputer, to communicate with a delicated multichannel scaler and a quadrupole mass filter. Via a digital input/output interface card and an AD/DA interface card, the experimenter may choose to take either a mass spectrum or a TOF spectrum, as the needs of the experiment dictate. Other mathematical manipulations of the acquired data can be easily implemented.

DESCRIPTION OF THE APPARATUS

In molecular beam spectroscopy a "universal" detector usually consists of an electron bombardment ionizer and a mass analyzer[2]. For mass analysis, a quadrupole mass filter combined with a channeltron can do the job very well. In the digital method, electronic instruments that can record the number of occurances of a given event in a set period of time (called the dwell time) are usually attached to this detection system. The instrument that we used is the Canberra Model 7880 fast multiscaler. It has a dwell time between 200ns and 1s and a built-in 4K 24 bit memory[3]. Because of its very short dwell time and high input count rates, it is particularly useful for applications in luminescence decay measurements and TOF spectroscopy.

For the quadrupole mass filter control, we have used the Extranuclear quadrupole controller (Model 011-1 quadrupole power supply and Model 4-324-9 quadrupole mass filter)[4]. There are two modes of operation. By varying the sweep voltage from 0 to 10 *V*, we can take the mass spectrum to determine what mass species are present. If we fix the sweep voltage to correspond to a particular mass, we can take the TOF spectrum and determine the translational energy of the particles.

Figure 1 shows the general arrangement of the experiment. An IBM PC XT compatible microcomputer was employed as the control center. Via a 12 bit D/A converter, the computer could control the mass analyser in either the mass sweeping mode or in the TOF mode. In the mass sweeping mode, the synchronization between the scaler and the quadrupole controller was achieved by sending both external clock pulses and a start pulse to the scaler via two lines of the 8255 digital interface card. The sweeping speed was controlled by a software routine. At the end of the routine, a mass spectrum was stored in the scaler and was ready to be transferred to the microcomputer. In the TOF mode, a specific mass was first selected and then fixed by the microcomputer through one D/A line. The internal clock was selected in the scaler and the TOF spectrum was taken and accumulated by the computer.

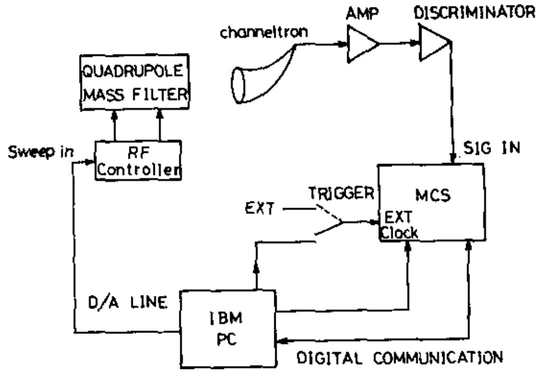

Fig. 1. Block diagram of the experimental set-up.

In summary the microcomputer controls the following processes: sending external start and external clocks to the CM 7880; varying the sweep voltage from 0 to 10 *volts* for the mass spectrum; fixing the sweep voltage corresponding to a particular mass for TOF spectroscopy; transferring data from CM 7880 to the microcomputer itself; and mathematically manipulating the acquired data.

CIRCUIT DESCRIPTION

Figure 2 shows the timing diagram between the CM 7880 and the IBM PC. A detailed description of the handshakes used in this interface is given below[3]:

(a) CON (Input from IBM PC): It must be always high when the CM 7880 is to transfer data to the IBM PC.

(b) ETI (Output from CM 7880): This is the interrupt signal that the CM 7880 sends to the IBM PC. It can hold up the CPU until the interrupt service routine for data transfer and signal averaging has been carried out.

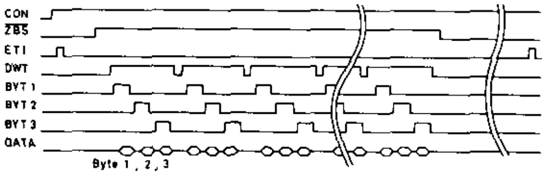

Fig. 2. The timing diagram of the CM 7880.

Table 1. 8255 interface configuration

Symbol	Name
PORT_1A	Input/Output port A
PORT_1B	Iuput/Output port B
PORT_1C	Input/Output port C
Ctrlreg_1	8255 Control register

(c) $\overline{ZBS}$ (Input from IBM PC): It must be held high when the CM 7880 transfers data to the IBM PC. If it is made low, the CM 7880 can not output data.

(d) DWT (Input from IBM PC): This handshake signal must be held high during data word transfer. The CM 7880 data word format consists of three bytes.

(e) BYT1, BYT2, BYT3 (Input from IBM PC): The three handshake signals control the transfer of the first data byte, the second data byte, and the third data byte, respectively. When held high, the CM 7880 outputs the corresponding data byte.

(f) D0, D1,…, D7 (Data bits): Each CM 7880 channel consists of three data bytes.

As mentioned previously, the interface between the CM 7880 and the IBM PC was achieved by an 8255 interface card. This interface card contains two 8255 chips. It is a general purpose I/O component for interfacing peripheral equipment to the microcomputer system bus. Each 8255 chip contains three 8-bit I/O ports and an 8-bit control register[5]. All of these could be configured with a wide variety of functional characteristics according to user's needs by writing control words to the 8255 control registers. For the present application, one 8255 chip is enough. Table 1 shows the specifications of the registers that we have used. Figure 3 shows the circuit diagram of the data and control lines of the present system.

PORT_1A, PORT_1B, PORT_1C are the data input/output ports. We utilized

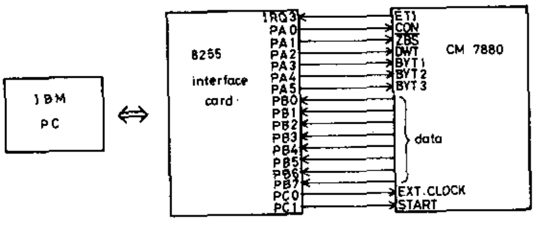

Fig. 3. Schematic diagram of the interface circuit

PB0-PB7 to accept data from the CM 7880; PA0-PA5 to send CON, $\overline{ZBS}$ DWT, BYT1, BYT2, BYT3; and PC0-PC1 to send EXT CLOCK and START to the CM 7880. As for ETI, we wire-wrapped it to the system interrupt IRQ3. The 12 bit DA converter was divided into two parts: the high 4 bit and the low 8 bit, each corresponding to different I/O addresses. By writting appropriate binary numbers for these I/O addresses, we can set the voltage for our quadrupole controller either to take a mass spectrum or do TOF experiments.

SOFTWARE DESCRIPTION

The software contains two parts: a main program written in FORTRAN language and three control programs written in 8088 assembly language. The flow chart of the FORTRAN main program is shown in Fig. 4.

The FORTRAN main program controls the experimental process according to the user's need. For example, before taking a TOF spectrum, one must determine the correct voltage for the quadrupole controller to control the quadrupole mass filter. This can be done by first taking the mass spectrum and then locating the

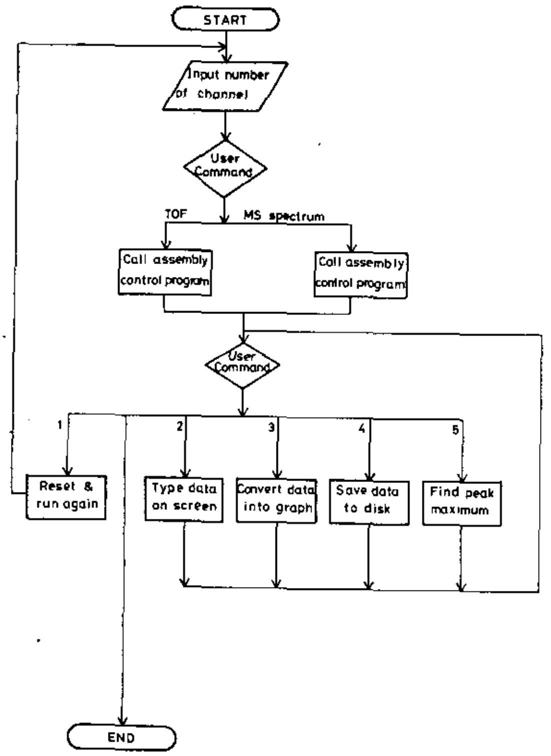

Fig. 4. Flow chart of the FORTRAN main program.

position of the peak maximum corresponding to the selected mass species. The appropriate voltage can be determined and sent out. After fixing the sweep voltage, one can proceed to take the TOF spectrum by just resetting the channel numbers and setting the number of repetitions (or scans) for signal averaging. The data transfer of either the mass or TOF spectrum and the signal averaging of the TOF spectrum are achieved by calling assembly subroutines. Through the main program the user can determine if he wants to take a mass spectrum or a TOF spectrum and the type data to be displayed on screen. The experimenter is able to convert the data into a graph[6], save data on a floppy disk, or find a peak maximum and set the sweep voltage, all with only a few keystrokes.

Three assembly control programs take care of the following processes: setting up input/output for chip 8255, setting up the 8259 interrupt handler for system interrupt IRQ3[7], masking the timer interrupt, sending EXT CLOCK and START to CM 7880, and sending the sweep voltage for the quadrupole controller. System interrupt IRQ3 is used by the interrupt service routine for data transfer and signal averaging executions. Signal averaging is achieved by adding data repeatedly to its corresponding channel number. The flow chart of the interrupt service routine is shown in Fig. 5.

Taking a mass spectrum is done by first sending START to the *CM 7880*. One then proceeds to vary sweep voltage from 0 to 10 V for quadrupole control and send EXT CLOCK to CM 7880 for channel advancing. The EXT CLOCK and sweep voltage must be sent with the appropriate timing to synchronize the multichannel scaler and quadrupole mass filter. The corresponding flow chart is shown in Fig. 6.

DISCUSSION

To accomplish the above tasks, several minor modifications were needed in the original hardware. First a change was required because the ETI interupt pulse was a little bit too short for the 8259 programmable interupt controller of the IBM PC resulting in irregular interrupting. To remedy this, a capacitor was added to the corresponding one-shot flip-flop of the CM 7880 to increase the pulse width to 15 microsecond, the minimum pulse width for a stable triggering of the IBM PC.

The second point deserving attention is that there is an error in the original timing diagram of the CM 7880 as offered by Canberra Inc. In the course of data transfer, DWT must always be high. If one just sends a short pulse for DWT, one will get the wrong result and not know what happened. With a TTL data book at hand and with a little thought about the hardware logic, one can find the error with little difficulty.

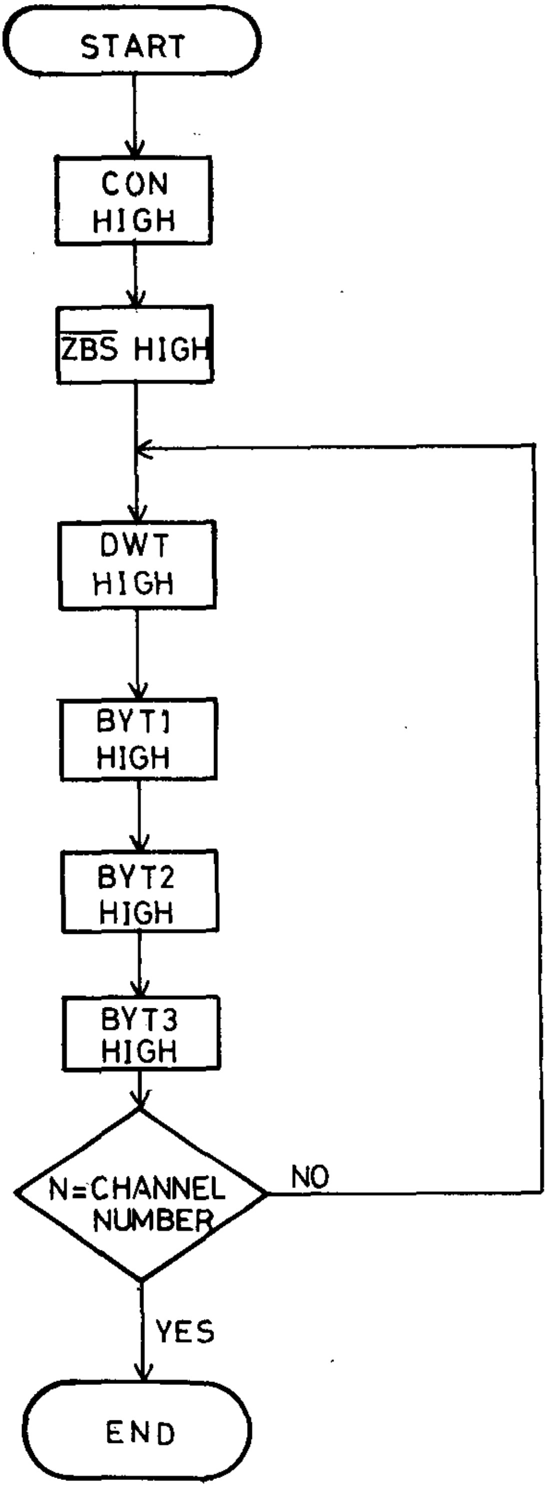

Fig. 5. Flow chart of the interrupt service routine.

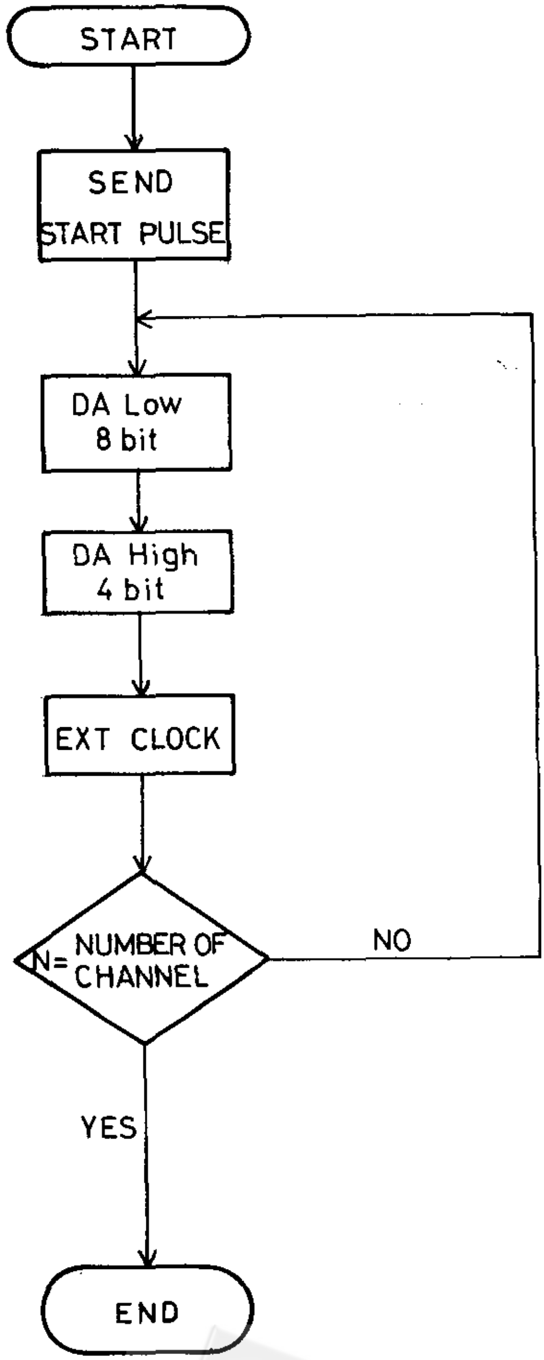

Fig. 6. Flow chart of the routine to control the taking of the mass-spectrum.

The third point is that the 8255 chip does not have enough current to drive the EXT CLOCK and EXT START ports of the CM 7880. A TTL line driver was added to boost the driving current of the 8255 chip.

The last problem was the ubiquitous DMA memory refresh cycles. The computer refreshes its memory every 72 clock cycles. When taking mass spectrum, the EXT CLOCK for the multichannel scaler is generated by software simulation using assembly language. The width of each clock pulse was affected by the DMA refresh cycle. This mades some clock pulses slightly longer than others and thus not predictable. It would make the dwell time of each channel slightly different. Fortunately, it takes time for a particle to pass through the quadrupole mass filter. If a too rapid sweeping were used, both resolution and signal strength would be degraded. We can neglect the effect of the DMA memory refresh if we increase the dwell time of each channel to be many times longer than the refresh cycle time, say 100 microsecond or longer.

As for the compatability of the hardware, an IBM PC, PC XT or PC AT or their compatible models are all equally suitable for the present interface system. Because of the plotting routines, the monocrome graphic card should be used for the microcomputers. Any quadrupole mass filter with built-in voltage sweeping capability could be easily adapted to the present interface system.

The software package with detailed operating instrutions and assembly programs is available upon request.

REFERENCES

(1) RCA Photomultiplier Manual, pp. 93-94, RCA Corporation, Harrsion, N.J. (1970).

(2) Y. T. Lee, J. D. McDonald, P. R. LeBreton and D. R. Herschbach, *Rev. Sci. Instrumt.*, **40**, 1402 (1969).

(3) CM 7880 Fast Multiscaler Instruction Manual, Canberra Inc., Meriden, CT. (1986).

(4) Quadrupole Power Supply Instruction Manual, Extranuclear Laboratories, Pittsburgh, Pa. (1979).

(5) Microsystem Components Handbook, Vol. 2, Intel Corporation (1985).

(6) The plotting routine we use is a modified Calcomp written by H. C. Lin. The Calcomp software package was originally developed for the Calcomp mechanical plotter. It can be adapted for use on an IBM PC.

(7) D. C. Willen and J. I. Krantz, 8088 Assembler Language Programming: The IBM PC, Howard W. Sams and Co., Inc. This book should be consulted for setting up the interrupt vector and for information on how to write an assembly program.

(Received August 25, 1987)