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A microcomputer system for mass spectrometer control and data acquisition

P G OZA, H S MAZUMDAR, A K CHOUDHARY and K GOPALAN*
Physical Research Laboratory, Ahmedabad 380009, India

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Abstract. A microcomputer system has been designed for semi-automatic operation of a solid source mass spectrometer used for geochronological studies. It sequentially steps the magnetic field through pre-selected values, reads the digitized ion currents for a given time and temporarily stores the data which can be transferred to a paper tape or directly to a desk top calculator for further analysis. The unit is relatively inexpensive, made of readily available components and can be adapted to many laboratory automation tasks.

Keywords. Mass spectrometer; data acquisition; microprocessor.

1. Introduction

A microprocessor based unit has been designed to control the magnetic field of a mass spectrometer for sequential peak jumping and to digitally store peak heights and baseline data for subsequent processing with an off-line computer. Besides being simple and relatively inexpensive it enables a single minicomputer to service many mass spectrometers. A similar unit using TTL-MSI logic was described by Dick (1975). The microprocessor used in the present design reduces the hardware complexities of a TTL-based circuit, and in addition provides for temporary data storage and if required, some simple data manipulation. Though designed for a semi-automatic operation of a solid source mass spectrometer for geochronological studies, it can be readily adapted or modified for many laboratory automation tasks.

2. Description of the system

The unit can step the magnetic field of a mass spectrometer sequentially through a maximum of 250 pre-selected values corresponding to peak and baseline positions. Since the isotopic analysis of most of the elements for geochronological studies requires not more than a dozen field values, the total number of channels can be grouped into independent blocks each storing the field patterns corresponding to commonly used mass spectra. It outputs a 16 bit binary word equivalent to 4 digit number in 1248 BCD format for each field value to the electromagnet supply *via* a high precision D/A converter. The output of the D/A converter in conjunction with base reference voltage selectable in the magnet supply serves to control the magnetic field either in the current mode or field mode using a Hall probe. Each field value is held at the parallel I/O ports,

* To whom all correspondence should be addressed.

under software control, for a preset 'delay time' selectable between 0·1 to 9·9 sec to allow the magnetic field to settle at the new value and thereafter, for a preset 'read time' also adjustable from 0·1 sec to 9·9 sec in steps of 0·1 sec to integrate the output of a voltage to frequency (V/F) converter corresponding to the ion current at the selected mass position. It can accumulate a maximum of 400 such data words (with the present memory capacity) with 7-digit precision, execute a chosen number of cyclic scans (up to 99) and at the end, transfer the stored peak height and baseline data in block format either to a teletype or directly to a desk top calculator through an IEEE 488 interface. A bank of 4 BCD thumbwheel switches in conjunction with a set of push-button switches enable front panel entry of the foregoing parameter for a given experiment (figure 2). A bank of 13 pairs of seven-segment LED's on the front panel display the pre-selected parameters and, in addition, the number of cyclic scans completed, the four-digit incremental field currently being supplied, to the magnet supply and the integrated V/F output except for the least significant digit, when the unit is in the RUN mode.

3. Hardware description

The system shown schematically in figure 1 consists of an Intel 8080 microprocessor with 2 kbytes RAM and 2 kbytes PROM. The other important hardware components are two Intel 8255 chips, one 8251 and one 8253, the choice being mainly to alleviate software complexity. Out of the total of six individually programmable 8 bit parallel I/O ports in the two 8255's, two ports (PAo-7, PBo-7) are used to supply the 4-digit field value in 1248 BCD format to the magnet control unit *via* a D/A converter. Two other parallel I/O ports (PC 1-7, PBo-7) are used for the 15 bit IEEE 488 interface with one bit from one of these ports (PCo) serving to open the gate for the two cascaded counters (Intel 8253) of 16 bit each for the preset 'read time'. Another I/O port (PAo-7) drives the cathodes of 13 pairs of LED display through a chain of decoders (2 × 7447) and display driver circuit. The last I/O port is divided into two parts of four lines each, one part ($PC_{4\text{-}7}$) being programmed in the input mode and connected to the horizontal rows of the thumbwheel and push-button switches. The other part (PCo-3) is programmed in the output mode and connected to a 4 to 16-line linear decoder (74154). Thirteen of the 16 decoded outputs drive the common anodes of the 13 LED pairs through an inverter chain (7404 × 3) and display driver circuit. Eight, out of the 13 lines, are common to these vertical columns of the push-button and thumbwheel switch array. Intel 8251 UART serves as a serial I/O port with 110 baud rate to communicate with the teletype ASR 33. This teletype was initially used in software development and later for data print out and loading any auxiliary programme separate from the permanent resident programme either by key entry or through paper tape. Two of the three individually programmable 16-bit counters in Intel 8253 have been cascaded to count the V/F converter output pulse train during the 'read time'. The third counter is programmed to divide the ϕ_2 clock signal at 2·04 MHz from the CPU clock generator (8224) to derive a signal at 1 msec interval to serve both as an external interrupt for the processor and as a clock signal for generating the preset delay time and read time. The oscillator signal at 18·432 MHz from 8224 clock generator is scaled down to 7·04 kHz through a divider chain (74161 × 3) and supplied to 8251 serial I/O port to generate the required baud rate of 110.

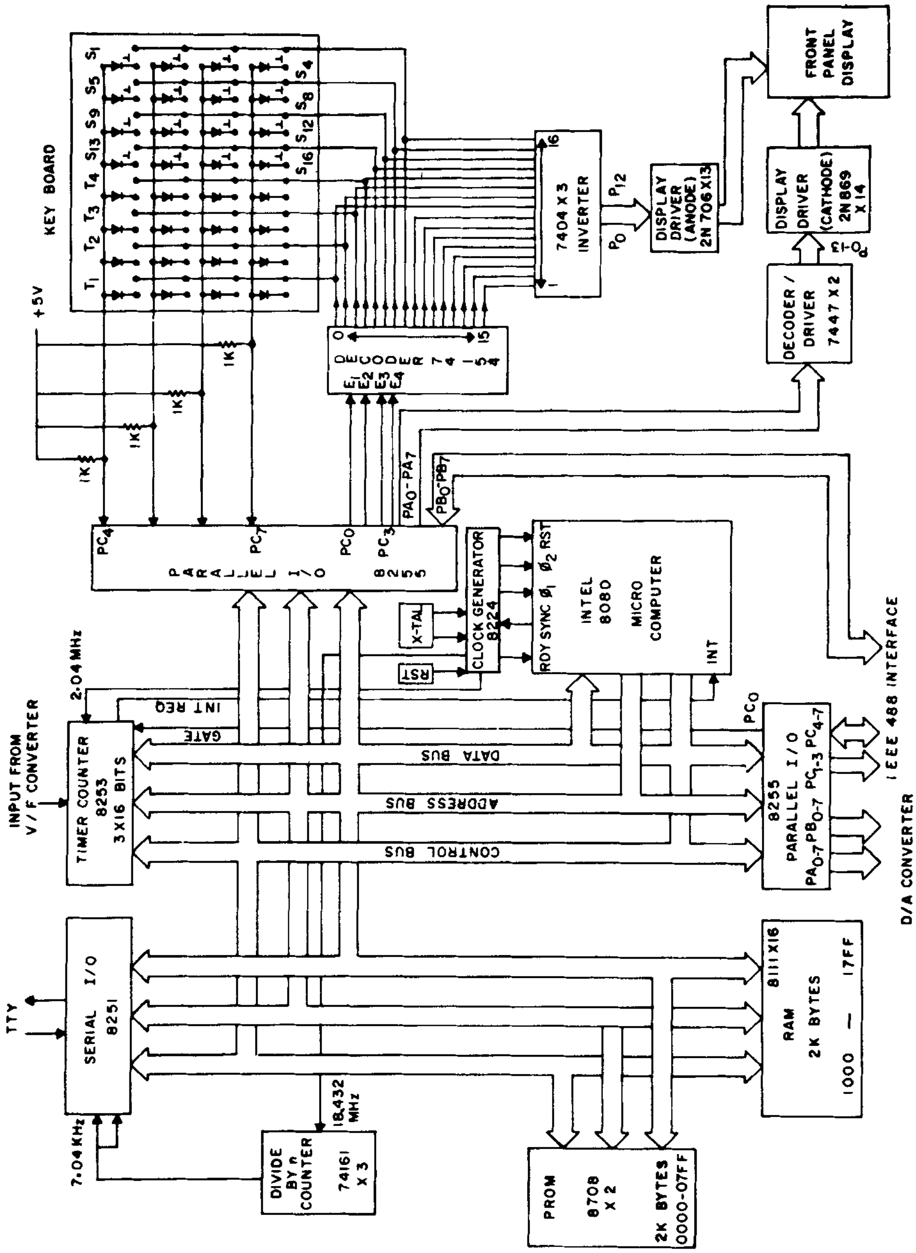

Figure 1. Schematic diagram of the microcomputer system implemented around Intel 8080 microprocessor with peripherals and communication interface.

4. Software description

The software has been developed in two independent packages, the background and foreground. The former supports the display and the switch array routines while the latter serves as the mother or the main programme. The switch and display array used in this unit require the microprocessor to be interrupted at regular intervals to scan the switch array to recognise any new entry and to update the display accordingly. The Intel 8080 microprocessor has been provided with a single interrupt vector. On every interrupt the CPU executes a RST 7 (restart) instruction causing the monitor to execute an unconditional CALL to RAM location (13 FD Hex) and initiate the programme called interrupt service sub-routine stored at that location. The CPU then returns to the operations it was performing before the interrupt had occurred. Thus the CPU is time-shared between the interrupt service sub-routine and the main programme. The background package keeps an image of switch array and display in memory and scans one column of the switch array at every interrupt to compare with the resident image to recognise any new entry. One complete scan of the switch and display arrays takes 16 msec to give a flickerless display. The mother programme has been written to incorporate the following features.

When the LOAD switch is activated, the LOAD sub-routine is executed which calls for the entry of an identification number for the block of channels to be used for a given element. The operator then enters the number of channels to be included in that block and then proceeds to enter the digital field values for each channel of the selected block. The programme stops at this point and the operator can recall the sequence for checking and editing, if necessary. Blocks of field patterns for other elements can be stored in a similar manner. The parameter entries are sequence-independent and protected against false entry.

On the first activation of the RUN switch, the RUN sub-routine is executed which calls for the entry of delay time, read time and the number of cyclic scans for the particular experiment for which the field pattern has already been stored. With the activation of the RUN switch again, the unit starts with the 4-digit field value in the first channel of the selected block, allows the delay time to elapse, reads the V/F output corresponding to

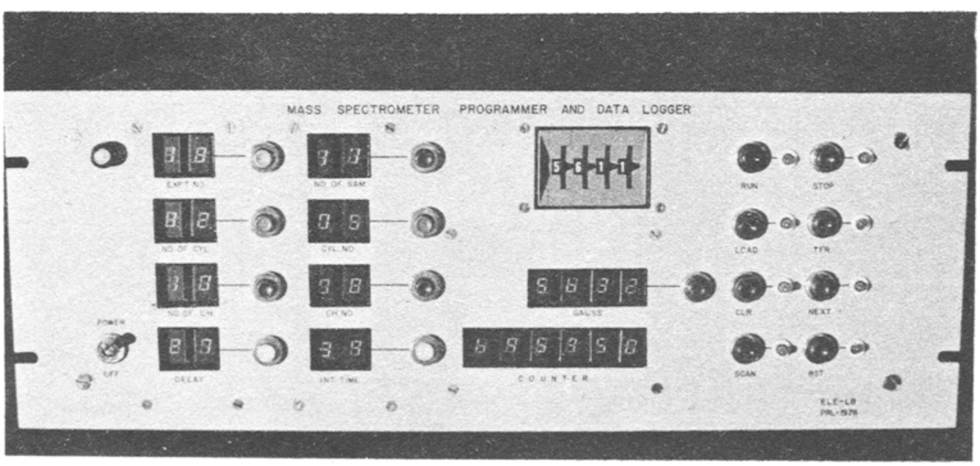

Figure 2. Front panel showing the switches for parameter entry and display.

the ion current intensity at the selected field position for the durations of the read time stores the accumulated value and then jumps to the next channel in the sequence. The repetition of the sequence stops at the end of the desired cycle.

The SCAN switch, initiates the SCAN sub-routine which calls for the entry of two 4-digit field values, delay time and read time. On activating the RUN switch now, the unit advances the field from lower value to higher value in unit steps, holding each field value for the duration of the selected delay time and read time. This scan feature allows the user to observe the profile of a mass peak in great detail.

All the subroutines branch off to ERROR subroutine whenever a wrong sequence of switches are used or a wrong entry is provided thereby terminating the erroneous operation. The ERROR subroutine brings about immediate lock out of the switch array and blinking of the display corresponding to the erroneous parameter for a delay time provided in the subroutine, after which the unit automatically recovers from the error hang up without losing the pre-stored parameters or data.

The TRANSFER switch enables the transfer of the stored data either to a teletypewriter or directly to a desk top calculator through an IEEE 488 interface, which at present is not included in the unit.

Any programme under execution can be temporarily halted for intermediate inspection and could be resumed by means of the respective function switch.

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Reference

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