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ELECTRONIC REDUCTION OF HIGH SPEED
MASS SPECTRAL DATA

J. R. LEE

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**ELECTRONIC REDUCTION OF HIGH SPEED
MASS SPECTRAL DATA**

J. R. Lee
Surface Physics Division 5114
Sandia Laboratories
Albuquerque, NM 87185

ABSTRACT

A window and peak height converter circuit has been designed and built that extracts a single mass peak (or group of peaks) from a set of mass spectra repetitive in time and produces a time profile of that mass. The response time of the circuit is such that one has the capability of real-time operation and of operation on mass spectral data that has been prerecorded on analog tape. The use of analog recording of data allows a great deal of flexibility in recording and playback speeds, and more importantly produces a permanent record of all information contained in the mass spectral data.

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INTRODUCTION

In past work on the reaction of atomic hydrogen with carbon,¹ serious problems were encountered in handling the large amounts of mass spectral data necessary to define the time course of this complex reaction. The UTI model 100C quadrupole mass spectrometer² used in our laboratory is capable of scan rates of approximately 6 msec/amu. Coupling this speed with a complex reaction such as that of atomic hydrogen with carbon, which produced 13 gas phase products ranging in molecular weight from 16 amu to over 120 amu, leads to the production of a prodigious quantity of data at rates so large as to preclude coupling to a digital device for data storage and reduction. Reducing the scan rates for recording of data on chart recorders, the method used previously,¹ of necessity ignores the majority of data potentially available.

Multichannel analog tape devices have an enormous capacity for data storage and are capable of recording such data at rates comparable to or greater than that necessary for our experiments, and moreover, gives the added flexibility of independently varying the record and playback speeds. Using the multichannel capability one can increase the dynamic range greatly by recording several channels at different gain settings. However, one still has the problem of extracting from this potentially huge amount of mass spectral data the time variation of a single mass peak or

group of peaks. An electronic solution to this problem can be built around the linear voltage ramp output from a quadrupole mass spectrometer. The frequency of this ramp is the repetitive mass scan frequency, and the relative mass position within a scan is directly proportional to the relative voltage amplitude within a single cycle. Concurrent analog recording of this ramp signal on a second channel of the same tape yields a voltage marker for each mass unit recorder.

We have designed and built a window and peak height converter circuit controlled by this concurrently recorded ramp signal. The window portion of the circuit is capable of passing the complete mass spectrum or any portion of the spectrum at any combination of mass scan rates and tape record or playback speeds. The peak converter portion of the circuit is capable of generating, again at any combination of scan rates and tape speeds, a continuous curve of the change in amplitude with time of a single mass species.

CIRCUIT DESIGN

The circuit given in Figure 1 was designed in three basic sections: (1) the window select section, (2) the position and width control section, and (3) the sample and hold section.

The window select section uses a window comparator that will generate output signals indicating when an input voltage (the 0 to 10 volt ramp from the mass spectrometer) is above, below, or between two independent and variable

reference voltages. The "go" signal from the comparator, which appears when the 10 volt ramp is between the reference voltages, is used to close a solid state switch and pass that portion of the mass spectrum corresponding to the ramp voltage between the reference voltages.

The position and width control section generates the two reference voltage levels for the window comparator. These levels are generated in such a way that once the lower level (width) is set it will be slaved to the upper level (position), keeping a constant width while adjusting the window position.

To generate the time profile of a single mass species, that portion of the mass spectra passed by the window select section is fed into the input of the peak detector in the sample and hold section. Both the peak detector and the sample and hold amplifier in this section are controlled by the output signals from the window comparator. The peak detector senses the maximum signal passed by the solid state switch during the period that the window is open. This maximum value is held by the sample and hold amplifier while the peak detector is reset for the next mass scan, and the value held by the sample and hold amplifier is maintained until replaced by a new maximum value from a subsequent mass scan. For sufficiently high scan rates the output of the sample and hold amplifier produces a continuous time profile of a single mass species.

CIRCUIT OPERATION

To illustrate the circuit operation the repetitive mass scan shown in Figure 2a was chosen. The mass spectrometers' 10 volt ramp output corresponding to the mass scan is shown in Figure 2b. The ramp first goes through a unity gain follower amplifier (IC5) for loading purposes and then into the input (E_i in Figure 1) of a window voltage comparator. The comparator compares this ramp to external voltages supplied to the lower limit set point (E_l in Figure 1) and the upper limit set point (E_u in Figure 1). The three comparator outputs (low, go, and high, Figure 1) produce the waveforms shown in Figures 2c-2e. The low output is generated when the ramp voltage is below the lower set point, the go output occurs when the ramp is between set points, and the high output indicates when the ramp is above the high set point.

The upper and lower set point voltage levels for the comparator are generated in the following manner: A voltage value of 0-10 VDC, depending on the setting of the position control potentiometer, is fed through a unity gain follower amplifier (IC4) to generate the voltage level for the upper limit set point (E_u in Figure 1). The width control potentiometer adjusts another independent 0 to 10 volt level. A differential amplifier (IC6) takes the difference of the two voltages and the new value is used as the lower limit set point (E_l in Figure 1). This method allows establishment of a voltage range corresponding to a mass width independent of the position on the mass scale.

The mass spectrometer signal (Figure 2a) is connected to one of the contacts on a solid state switch (IC3, Figure 1). The "go" output from the comparator closes the switch passing that portion of the mass scan chosen by the position and width control section. Figure 2f illustrates the result of a 1 amu width centered at mass 16 amu.

To produce a continuous curve of peak amplitudes as a function of time, the output of the solid state switch is fed into a peak detector (Burr Brown 4085 KG, Figure 1). This peak detector has three modes of operation: peak detect mode, hold mode, and reset mode. Logic inputs A and B select the mode of operation according to Table 1a. The comparator outputs, "low" (Figure 2c) and "go" (Figure 2d), are inverted (IC1) and fed into logic input A and B, respectively, so that when the ramp is below the lower set point on the comparator, the peak detector will be in the reset mode and set its output to 0. When the ramp is between set points, the peak detector will be in the "peak detect" mode. While in this mode, the peak detector output will follow the input until a maximum value is reached, and hold this value for the remainder of the peak detect portion. The ramp now goes above the upper limit set point and the logic inputs will put the peak detector into the "hold mode," holding the maximum value regardless of the input. Repetition of this cycle generates the waveform shown in Figure 2g as the output of the peak detector. This signal is fed into a sample and hold amplifier (IC2) controlled

by the "high" output from the comparator. Table 1b contains the sample and hold amplifiers truth table. When the peak detector has found the maximum value of a peak and is in its hold mode, the high output signals the sample and hold amplifier to sample that value. At the end of the high portion of the cycle, the sample and hold amplifier holds this value until signaled by the window comparator on the next cycle to sample a new value. The resulting output of the sample and hold amplifier is the stair step curve in Figure 2h. For sufficiently high cycle frequencies, this will generate a smooth curve.

CIRCUIT PERFORMANCE

The data in Figure 3 illustrates the performance of the window and peak height converter circuit for realistic data. From past experience, it is known that the introduction of hydrogen into an ultra high vacuum chamber will cause an increase of peak heights for masses other than those of hydrogen. Knowing this, a set of mass spectral data was recorded continuously on tape before, during, and after hydrogen was introduced into the vacuum chamber. The mass spectrometer scan range was set to cover masses 10 through 45 with a speed of approximately 6 msec per mass unit.

Replaying the tape at a much slower speed, a single scan (Figure 3a) was chosen approximately 5 seconds before hydrogen was introduced. Figure 3b shows a second single scan from

this set taken approximately 10 seconds after hydrogen was introduced. Comparing the two scans, it is seen that a reaction has indeed taken place, producing a large array of mass peaks. For the purpose of demonstrating the window and peak height converter circuit the details of this reaction are not important.

Replaying the data into the window and peak height converter circuit at a tape speed equal to the recording speed, masses 15, 28 and 18 were chosen and each followed throughout the experiment (Figures 3c, 3d and 3e). From inspection of the mass spectrum in Figure 3b, one concludes that these mass peaks probably result from separate chemical species: mass 15 from CH_4 , mass 28 from CO and mass 18 from H_2O . Comparing the three curves, it is seen that the time variation of all three mass peaks are different, supporting the contention that each results from different species. For a more complete identification of the species involved in the reaction, one would compare time profiles and relative amplitudes for a larger number of mass species. Correlations could then be made according to known mass-analyzer "cracking patterns."

CONCLUSION

The large amounts of complex mass spectral data encountered in past work necessitated the development of a method of extracting information contained in such data. The system described here is capable of selecting any mass peak in the spectrum and generating a continuous curve of the change in amplitude with time of that mass peak.

The window and peak height converter can be used directly with the mass analyzer at any scan frequency or with data previously recorded on a multichannel analog tape recorder, the use of such an analog recorder allows one to permanently record huge amounts of mass spectral data and have the added flexibility of independent record and playback speeds. To illustrate the storage capacity of the tape deck, approximately 4000 mass peaks were recorded during a 40 second time period as described in the circuit performance section. If the full length of tape were used (9200 ft.) and three separate channels recorded concurrently at different gain settings, the maximum capacity of this system would be approximately 4 million mass peaks over a period of four hours (at a tape speed of 7½ ips). The present system would allow one to recover the complete time profile of any selected mass peak from such a mass of data in about 15 minutes. The storage capacity of this present system is limited only by the frequency response of the analog tape system.

Other uses of the window and peak height converter would result from paralleling several units. The most obvious would be simply plotting several mass peaks simultaneously on a multipen recorder, but by multiplexing the outputs, one could also follow several different mass peaks simultaneously to monitor realtime system performance. By the addition of a simple variable subtraction circuit, one could partially process the raw data. For example, it might be desirable to subtract the contribution at mass 16 (mass 16 is common to several

molecular species) due to CO_2 . For this, the peak at 44 would be attenuated by the ratio of 16:44 in the cracking pattern of CO_2 and subtracted from the experimental peak at mass 16. Similarly, one could construct an analog divider circuit to ratio two experimental peaks. The consistency of such a ratio can be used as a test of constant product distribution and the magnitude of the ratio used to identify species from known cracking patterns.

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REFERENCES

1. R. R. Rye, Surface Science 69, 653 (1977).
2. Uthe Technology International, Sunnyvale, California (Model 100C Precision Mass Analyzer).

TABLE I

a) PEAK DETECTOR TRUTH TABLE

	logic input A	logic input B
peak detect mode	1	0
hold mode	0	0
reset mode	0	1

**b) SAMPLE AND HOLD AMPLIFIER
TRUTH TABLE**

	sample hold control
sample mode	0
hold mode	1

logical 0 = .8volts or less

logical 1 = 2.4volts or greater

Figure 1. Window and peak height converter - schematic diagram.

Figure 2. Waveforms at various stages of the window and peak height converter. a) Mass spectrometer output. b) Mass spectrometer ramp output. c) Window comparator "low" output. d) Window comparator "go" output. e) Window comparator "high" output. f) Window output. g) Peak detector output. h) Sample and hold output.

Figure 3. Circuit performance. a) Single mass scan 5 seconds before the introduction of hydrogen (hydrogen introduced at 10 seconds). b) Single mass scan 10 seconds after the introduction of hydrogen. c) Time profile of mass 15. d) Time profile of mass 28. e) Time profile of mass 18.