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MICROCOMPUTER-MULTICHANNEL ANALYZER DATA SYSTEM
FOR FOREGROUND-BACKGROUND DATA COLLECTION AND ANALYSIS
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ABSTRACT

A microcomputer-multichannel analyzer (MCA) system was assembled to obtain
foreground-background performance in data collection and analysis for x-ray
photoelectron spectroscopy. The MCA performs pulse counting analysis, while
the microcomputer is free to evaluate previously down-loaded data or perform
other computing functions. No special interfacing hardware is required beyond
single digital to Analog (D/A), and Analog to Digital (A/D) converters.
Analysis and computing time is optimized with a minimum interfacing expense.

INTRODUCTION

Data acquisition systems for x-ray photoelectron spectrometers (XPS) have
followed an evolutionary path somewhat analogous to that of the spectrometers
themselves. Like their laboratory-built predecessors, the first commercially
produced spectrometers had relatively simple but efficient data acquisition
based on pulse-counting and multichannel-scaling with a multichannel analyzer.
As commercial spectrometers evolved into complete multi-instrument systems, the
data acquisition also became more sophisticated, with the use of minicomputers
for both acquisition and analysis of data. However, a relatively powerful and
expensive computer is required to do both acquisition and analysis in parallel,
usually referred to as a foreground-background operating system. With sophisticated programming, an inexpensive microcomputer can be made to operate in a foreground-background mode, but the relatively slow logic (typically 4 MHz) results in virtually all the processor time being assigned to pulse-counting. The purpose of this communication is to show that by taking an evolutionary step back, in a sense, and again using a multichannel analyzer for the pulse-counting operation, the MCA can be slaved to an inexpensive microcomputer to produce a very powerful data system operating in a foreground-background mode.

The micro-computer for the approach described here may be of the users choice, with additional options for data storage and output to fill the requirements of the experiments. The hardware requirements of the computer for interfacing are one D/A output and one A/D input. The multichannel analyzer must have the capability of driving the analysis by simultaneous voltage ramp output during data acquisition. The multichannel analyzer must also have an electronic switch for external activation of data output. In addition, the ability to view the data during collection is advantageous.

SYSTEM COMPONENTS

The x-ray photoelectron spectrometer used is a Physical Electronics 548 ESCA/Auger system. The output from the photoelectron detector is amplified by an Ortec 547 amplifier, converted to TTL pulses by an Ortec 536 discriminator, and then counted by a Tracor Northern 1706 multi-channel analyzer. Data is displayed on a Tracor Northern 1314 display unit. The micro-computer in this system is an IBM-PC.
Figure 1 is a block diagram of the data collection system. Data acquisition is initiated by a front panel switch on the TN-1706. During data acquisition the TN-1706 outputs a 0-5 volt ramp which drives the Physical Electronics 11-055 ESCA-Auger system control. The Physical Electronics 11-055 and 20-805 constitute the control circuitry for the CMA analyser in both Auger and XPS detection modes. Ramp output from the 11-055 to the 20-805 is converted into the analyzer voltages required to obtain the desired scan. The pass energy, modulation, and detection mode (XPS or AES) are controlled by the 20-805. Sweep limits and rate are controlled by settings on the 11-055. The 11-055 internal ramp circuitry is by-passed by a rear panel switch, while retaining control of the starting binding energy and sweep range. The data collection sweep rate (millisec./channel) is set on the TN-1706, (the MCA sweep rate selection also controls the rate at which data is output).

Signals from the XPS analysis follow the path shown in Fig. 1. After amplification of the multiplier pulses, a discriminator removes any signal under a pre-set amplitude. The discriminator level was set such that no counts were detected when photoelectrons were not being generated. A rate meter is included in the system to maintain the count rate below the limits of the spiraltron detector in the spectrometer. The accumulated spectrum in the memory of the TN-1706 may be observed on the TN-1314 display screen. Data collection may continue until acceptable signal to noise is attained.

Down-loading of the collected spectrum is initiated by the change in a voltage level to the TN-1706. The initial voltage level of +5 volts is set at the start of the data collection/analysis program, inhibiting the possibility
of data output during data collection. One subroutine in the data collection/analysis program performs the voltage change and the A/D conversion of the data from the TN-1706. At the beginning of this subroutine, the D/A voltage level is switched to initiate the output of analog data from the TN-1706. The change in voltage is accomplished by loading a new value into the D/A converter address. Immediately upon completion of the D/A command the data collection subroutine begins the A/D conversion of the 512 data points. Serial ASCII output from the TN1706 is also available, although to utilize this input mode, an additional input port card would have to be purchased. In principal, direct digital transfer would be preferred. However, errors of <1% in analog data transfer and conversion are acceptable, making the added expense unnecessary. The TN-1706 data output rate is set to 40 milliseconds per channel, only a fraction of which is required for the analog to digital conversion. A time wasting loop is placed in the conversion portion of the subroutine to synchronize the conversion rate to the output rate. A schematic diagram of the logic of the data collection subroutine is shown in Fig. 2. Upon completion of the A/D conversion, the data are converted to count values by multiplying the result by:

\[
\text{Counts} = Y(i) \times \frac{VDS}{2048}
\]

where: \( Y(i) \) - is the result of A/D conversion for the \( i \)th point

\( VDS \) - is the vertical display scale of the MCA,

\( (# \text{ counts full scale}) \)

2048 - is the number of A/D conversion channels

The spectrum, along with the description of the specimen and analysis conditions are recorded upon magnetic disk following the completion of the data
transfer. The TN-1706 is now free to collect another spectrum, while the operator may interpret the previously collected data on the computer.

The XPS data analysis program is a simple non-iterative curve fitting routine which uses a Gaussian lineshape and an s-shaped background. Smoothing of the spectrum, and Mg Kα₃,₄ satellite removal may be performed before fitting of the photoelectron peaks. Results of the data analysis include the area under each peak and the standard deviation of the fitted curve from the experimental results. Hardcopy of the data is obtained which shows the fitted line over the collected spectrum as well as the contribution of each peak. An example of this output is shown in Fig. 3.

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FIGURE CAPTIONS

Fig. 1. Block diagram of the data collection system illustrating the connections with the micro-computer.

Fig. 2. Schematic of the data collection subroutine.

Fig. 3. Example of data collected and analyzed by the multi-channel analyzer, micro-computer data system.
Fig. 1
Data Collection Subroutine

1. Enter Specimen Description and Analysis Conditions
2. Enter Vertical Scale, (VDS) from MCA, Counts Full Scale
3. Set D/A = 0.0V
   Begin Output
4. For 512 Data Points
   Y(I) = A/D Conversion Result
   Time Wasting Loop
5. Convert Y(I) to Count Values
6. Plot Results
7. Return to Main Program
Specimen: GOLD FOIL

Analysis Conditions: 300 W MG 50 EU PASS 1.6KV MULT AU(4F)

Fig. 3

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