P. M. Grant

Automation of a Wide-range, General-purpose Spectrophotometric System

Abstract: The application of an IBM 1800 computer to the control and data acquisition functions of a wide-range spectrophotometric system is described. The optical part of the system is designed primarily for solid-state spectroscopy in the reflectance mode, the energy range of interest being roughly 1 to 12 eV (10^4 to 10^5 cm^{-1}). The operations of the computer include regulation of the wavelength setting, determination of the system gain, analog-to-digital conversion of the output signal, and positioning of the sample and detector. Two experimental configurations are employed, depending on whether or not the sample and detector are to remain stationary or to be repositioned during a run. The former holds for electroreflectance, fluorescence, and photoconductivity studies, while the latter pertains to ordinary reflectance and transmittance measurements. The principal advantage to be derived from on-line computer control of such experiments, besides more rapid accumulation and reduction of data, is the improvement in signal-to-noise ratio by averaging many repetitive scans over the same energy range. The emphasis in this paper is on the software used to implement these operations.

Introduction

Much of what is known today of the electronic structure of solids has been revealed by study of their optical properties in the visible, ultraviolet and infrared spectral regions.[1] The optical response of a material can be measured in several different ways. Probably the most common and widely used technique is simply to shine light through a given sample and record the absorption as a function of wavelength. All materials, however, begin to absorb heavily at some wavelength, necessitating the preparation of ultrathin and perhaps ill-characterized samples. In recent years, the use of normal and nonnormal incidence reflectivity has grown rapidly as a tool to investigate optical properties in these highly absorbing regions. Even more recently, variations on these techniques in the form of modulated optical response measurements have appeared.[2] Here one impresses an undulating pertubation on the sample such as electric fields, stress, magnetic fields, temperature or some combination thereof. One then performs coherence detection of the transmitted or reflected light, thus observing the effects of the perturbations on the electronic states of the solid at a reasonable signal-to-noise level. Such techniques can also be applied to the various optical rotary and birefringence effects. For example, the polarization of the incident light energy can be modulated, thus facilitating measurement of Faraday rotation, polar Kerr effect, and the like.

The author is at the IBM San Jose Research Laboratory, San Jose, California.

Equally useful for electronic structure studies is the manifold of phototransport phenomena. These are typified by the well-known photoconductivity and photovoltaic effects whose response as a function of incident light energy complements information derived from purely optical approaches.

This interest in the optical properties of solids has spurred the development of many and varied types of spectrophotometric instruments in both industrial and university laboratories. In this paper, we discuss the use of a digital computer connected to a wide-range optical spectrometer in a configuration suitable for many of the studies outlined above. As a prelude, however, let us examine some of the general problems of spectrophotometer design.[3] The ones that would involve computers fall into three general classes.

(1) Each source device in an optical spectrometer has a spectrum of its own which must be accounted for in the measurement of the sample response. That is, one has to record, at a given wavelength, the light intensity incident upon the sample as well as the intensity reflected from it (or transmitted through it or the photocurrent in it, as the case may be) to obtain an absolute measurement.

(2) Often one desires to catalog large amounts of data, either from various samples in the same wavelength range, or from the same sample over different wavelength ranges. For the latter, it is usually desired to eventually concatenate the data into a single spectrum. Also, it has

become necessary with increasing frequency to treat data with sophisticated analysis techniques to extract the underlying physics. Thus the means by which the spectrophotometer presents its output to the experimenter has high significance.

(3) Noise problems in spectrophotometric apparatuses have always received much attention and will become even more important to solve as interest in the optical properties of solids proceeds to increasingly subtle effects.

Each of the above design considerations has been attacked by well-known procedures. Manufacturers of commercial absorption spectrometers use a method for normalizing the sample response with respect to the source spectrum whereby the incident light is switched between two channels, one containing the sample and the other either empty or holding a reference. The two beams of light are then focused on a detector in which the associated electronics produces their ratio. However, there are several areas in which this technique is difficult to apply, some examples being magneto-optical measurements in high fields, vacuum ultraviolet reflectivity, and particularly the measurement of reflectivity at different angles of incidence. For such cases, two scans over the same wavelength range, one with the sample removed and the detector intercepting the incident light beam, and the other with the sample interposed, provide the data with which to calculate the normalized optical response. On the other hand, it should be mentioned that the several ingenious methods of measuring modulated optical response have reduced the importance of the double-scan approach.[2]

Point (2) requires that data be retained in graphical form, or at least in terms of line-shape parameters. This is usually effected through a strip recorder device connected to the output of the detector amplifier. Also, point (2) demands that these graphical data be reduced to unit record computer input. For large quantities of data, these considerations soon give rise to serious tedious and time-consuming problems.

The most universal approach to noise reduction has been to use some form of coherence detection in conjunction with *RC* time averaging. One common method is to mechanically modulate the incident light at a constant frequency and employ a phase sensitive detector, or lock-in amplifier, to enhance the signal produced by the light detector. The desired low frequency sideband is then obtained by passing the output of the phase sensitive detector through a low-pass *RC* filter. As the noise level increases, compensating increases in the *RC* filter time constant and scan period are made. This method, however, is not as effective against low-frequency noise as the one to be discussed here.

Application of on-line digital computer control to a spectrophotometric system will yield solutions in each of the three areas under discussion. As mentioned, there are still some experiments in which double scan operation is desirable. Although sample-detector manipulation is most conveniently performed by the computer through electromechanical devices, this function can be handled manually. Much more important is to have access to the computer for the data-logging function inasmuch as it is here where the greatest reduction in labor is afforded. Thus, in the development of the system described in this paper, lowest priority was given the sample-detector movement problem and greatest attention directed toward data conversion and storage. Having the data available within the computer greatly facilitates ratio calculations and concatenation with results from other energy ranges. In addition, it almost always is desired to analyze these data either in terms of some physical model or else reduce it to more elemental form. An excellent example arises in the use of the Kramers-Kronig transform to produce optical constants from reflectivity data. These derived data are sometimes merely catalogued, but often it is needed for testing of a given theory. In any event, being able to manipulate data within or among computer systems without manual transcription is a worthwhile goal of spectrometer automation.

Perhaps, however, the greatest reward comes from using the computer to increase the confidence level of the data and thus improve the quality of experimental physics being undertaken. This can accrue from merely being able to repeat the experiment two or three times, whereas the previous cost in data reduction labor would have discouraged such practices. In fact, it now becomes possible to repeat the measurements many times and apply time averaging to reduce noise. The efficacy of time averaging, that is, repeating the experiment many times over the same wavelength range and averaging results, *vis-a-vis* single scans with long integrating time constants, has been examined by Ernst.[3] Under the assumption that the *total* time available for a given experiment is fixed for both time averaging or single scan mode, his conclusions may be summarized as follows:

(1) If the noise present in the signal has a uniform power spectral density (white), both methods result in the same signal/noise ratio.

(2) If, however, the noise power spectral density behaves as f^{-m}, $0 < m \leq 1$, time averaging is superior to single scanning. This is the density function which describes the shape of the noise spectrum usually found in spectrophotometric systems.

(3) In both cases, the signal/noise ratio improves as the square root of the number of scans in the time averaging mode.

By providing the means to repeat and store a measurement many times, the computer thus becomes the principal

tool of the experimenter in allaying noise problems. It is even possible to have the computer analyze the noise pertinent to a given experimental situation and then construct its own "filter" against it.

In the sections to follow, we describe the experimental apparatus, the computer interface, and, in some detail, the software package which has been created to run general optical experiments, the illustrative example being reflectivity. Finally, some experimental results will be discussed in reference to those points brought forth in the present section to which computer assistance has been applied.

Experimental apparatus

The heart of our optical system is a 1/2-m focal length McPherson Model 235 monochromator of the Seya-Namioka type. With the proper choice of source and detector, this instrument can operate over the energy range 1 to 20 eV with resolution sufficient for most applications in solid-state spectroscopy. The salient optical parameters are summarized in Table 1, and the over-all optical path is shown schematically in Fig. 1. Although designed primarily for operation in the reflectance mode, the system has also been used for photoconductivity and photovoltaic studies as well as electroreflectance and transmittance measurements. Because, however, our scientific interests presently center on the intrinsic optical properties of materials (those energy regions where solids absorb light heavily), the discussion will be carried on in reference to reflectance.

As seen in Fig. 1, light incident on the plane of the sample surface is intercepted by the detector in either one of two positions. If the sample is removed from the plane of incidence, the detector is placed in the I_0 position for measurement of the incident light energy. The sample is then interposed and the detector rotated to a position (I_R), depending on the angle of incidence. In actuality, the detector is an aluminum-coated quartz light pipe in the shape of a question-mark which feeds the signal to a photomultiplier tube situated outside the sample chamber.[5] The sample itself is held on a liquid-nitrogen dewar cold finger which can be moved in and out of the beam and rotated for reflectance studies at different angles of incidence. Both sample and detector devices are controlled through the computer by small dc motors.

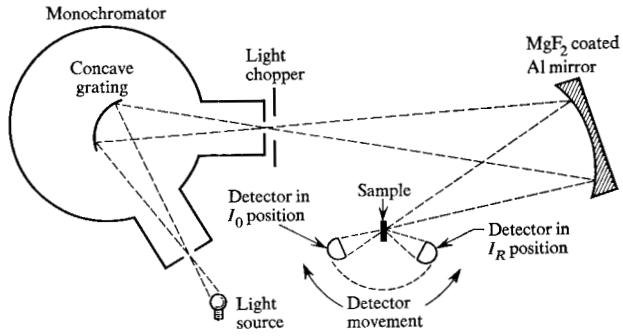


Figure 1 Schematic of the optical system. Monochromatic light emerging from the monochromator exit slit is chopped by a tuning fork device and is focused by a mirror set slightly off-axis with demagnification of two onto the sample. The dectector is rotated on-axis about the sample between the I_0 and I_R positions.

Table 2 Sources and detectors for various spectral ranges.

Spectral range	*Source*	*Detector*
1.2 μ-6000 Å (1–2 eV)	Tungsten lamp	RCA 7102 PMT
6000–3500 Å (2–3.5 eV)	Tungsten lamp	EMI 6256S PMT
4000–2000 Å (3–6 eV)	High pressure deuterium lamp	EMI 6256S PMT
2400–1700 Å (5–7 eV)	Discharge lamp—hydrogen continuum	EMI 6256S PMT Light pipe overcoated with sodium salicylate
1700–1200 Å (7–10 eV)	Discharge lamp—H and Ar line spectrum	Same as 2400–1700 Å
1200–600 Å (10–20 eV)	Discharge lamp—H, He, and Ar line spectrum (windowless operation)	Same as 2400–1700 Å

Table 2 gives an indication of the source-detector combinations needed to cover the range 1 to 20 eV. The pertinent point is that each of these combinations produces scan data which must be saved by the computer for later concatenation with other ranges. We note that in the vacuum ultraviolet region (above 6 eV) light is absorbed

Table 1 Various parameters of the optical system.

Grating	*Blaze*	*Wavelength range*	*Dispersion*	*Aperture*	*Nominal slit width*	*Light power incident on sample*
300 lines/mm	5000 Å	2000–12000 Å	66 Å/mm	$f/17$	100 μm	10^{-2} μW @ 5000 Å
600	1500	500–3000	33	$f/17$	100	10^{-4} μW @ 2000 Å

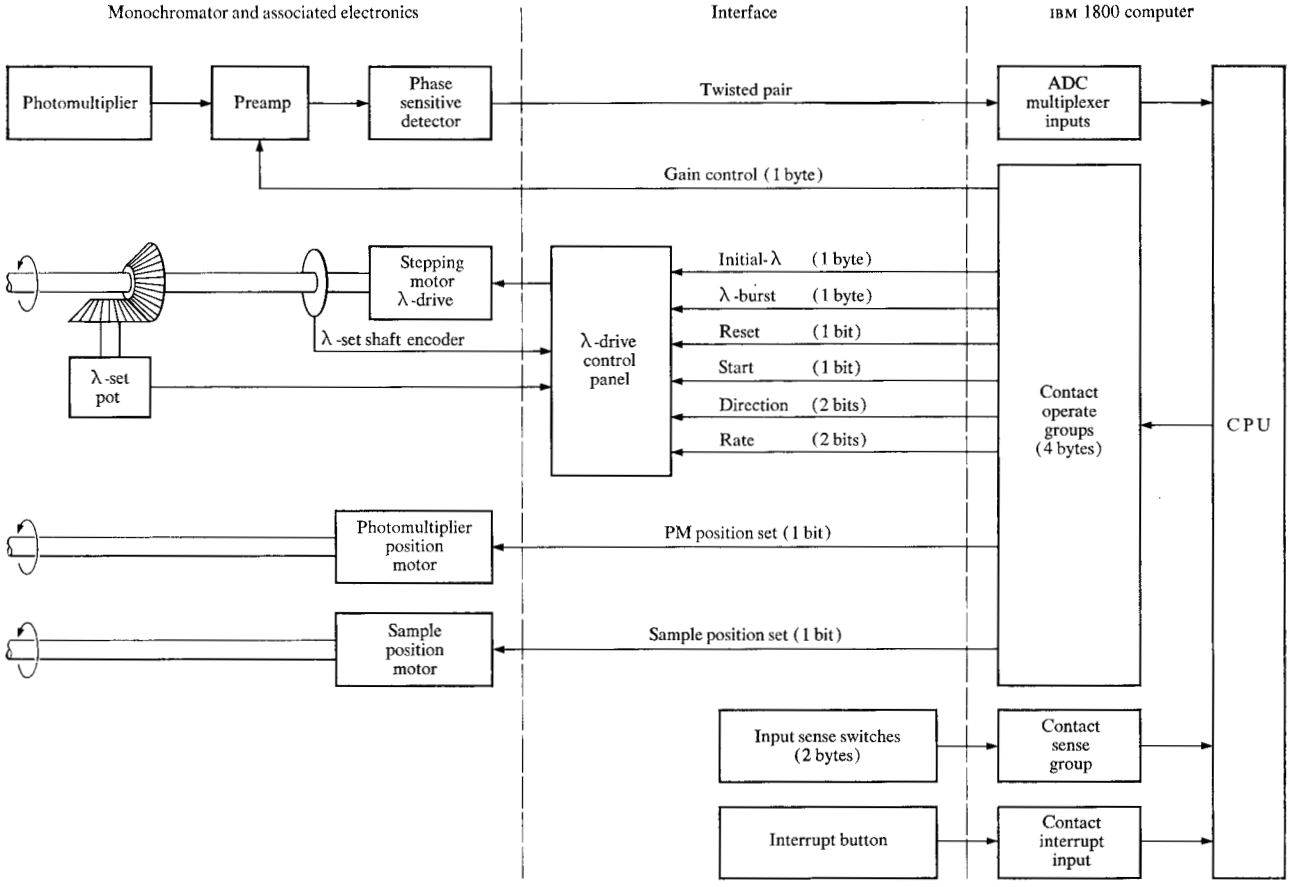


Figure 2 System block diagram indicating the hardware linkage between the spectrophotometer and the computer. Altogether one ADC input, two contact operate groups, one contact sense group, and one contact interrupt are used in the connection. A contact operate group is a 16-bit word comprised of 16 solid-state relays into which the computer can write so as to control external electromechanical devices. A contact sense group is a 16-bit word read by the computer, each bit being set by an external contact closure.

Table 3 Hardware configuration of the IBM San Jose Research Laboratory computer installation.

Word length	16 bits	I/O devices	1442 card reader/punch 1443 line printer
Core size	32 K		Keyboard Typewriters (4)
Core speed	2μsec		Calcomp plotter
Number of disks	3	Analog/digital I/O devices	32 high-level analog inputs (0–5 V)[a] 32 low-level analog inputs (±50 mV)[b]
Total disk capacity	1500 K		16 analog outputs (0–10 V, ±10 V) 6 contact sense digital input (16 bits)
Timers	0.125 msec 1.000 msec 8.000 msec		2 voltage sense digital input (16 bits) 13 contact operate digital output (16 bits) 3 pulse digital output (8 bits)
Interrupt levels	24	ADC & multiplexer	44 μsec conversion time Model 2
Interrupt terminals	64 contact sense 32 voltage sense	Data Channels	9

[a] Solid-state multiplexed, single ended.
[b] Relay multiplexed, differential.

heavily by the ambient atmosphere so that the entire experimental apparatus must be evacuated.

The over-all system is considered as comprised of the three parts shown in Fig. 2. The hardware attributes of our process control computer installation are given in Table 3. The photomultiplier output is fed to an operational amplifier whose gain is set by the value of the feedback resistor inserted under relay control by the computer. The signal then continues through the usual phase-sensitive detector processing, becoming converted to a dc signal which is fed to one of the low-level analog-to-digital inputs of the computer. The signal is also monitored in the laboratory on a strip chart recorder. The wavelength setting is controlled by devices similar to those described by Hannon, Horne, and Foster,[6] and the reader will find the details discussed therein (our system differs slightly in that a 10-turn potentiometer driven by the stepping motor through a gear reduction box is used to set the initial wavelength instead of an internal spectrometer slidewire). In addition, sample-detector positioning is handled as shown, the sign of the contact operate bit determining the direction of rotation of the motors. As well as providing a means for the computer to control and receive data from the apparatus, provision must be made for the experimenter to communicate (preferably from his laboratory) with the machine for the insertion of appropriate run data. For this function, a contact sense (CS) input word (2 bytes) is connected to a bank of 16 toggle switches in conjunction with the use of the contact interrupt (CI) feature of the computer.

Experiment-controlling software considerations

The 1800 operating system, to which all subsequent programming discussions will be in reference, was designed and programmed within the IBM-supplied Time-Share Executive (TSX) package by H. M. Gladney.[7] In this paper we will refer to the operating system as TSX-GEM (for General Experimental Monitor), and the reading of Ref. 7 is an essential prerequisite for understanding what follows. In order to provide a frame of reference for our discussions, we have summarized the relevant features of our computer system and the TSX-GEM operating system in Table 3 and Fig. 3, respectively.[8]

When the performance of a spectrophotometric measurement is analyzed, it divides naturally into two phases: The run initialization phase, where the various scan parameters such as wavelength interval and scan speed are decided upon and set, and the data acquisition phase, in which the scan is set into operation and the data logged. This is shown schematically in Fig. 4. Tied to the contact interrupt button is a small program, loaded into core at each interrupt displacing the job under operation, whose function is to read the contact sense switches and store their contents on a small file on disk. The flow chart for this program is shown in Fig. 5.

The program itself is initialized by clearing the CS switches and depressing the CI button. This action sets the run parameter counter stored on disk to unity. Also, during the run initialization phase, the contact operate (CO) group that sets the initial wavelength and gain during the acquisition phase is used to indicate in panel lights the contents of the run parameter counter, so that the experimenter may know which data to enter next. That is, the operator enters the run parameter quantity requested by the CO lights into the CS switches and depresses the CI button. When he sees the CO lights updated by one, he knows the quantity has been accepted and stored, and may proceed to put the next one into the CS switches. When the appropriate number of run parameters has been entered for the particular task in question and the data acquisition phase is to be commenced, the CS sign bit (8000_{16}) is turned on and the CI button pressed once more. Thus the entire task of communicating the data necessary for a given experiment to the computer *has taken place completely within the laboratory through the use of a simple set of lights and switches in an open-ended manner.* An IBM 1053 printer was later added for the purpose of obtaining more comprehensive output from the computer, and for validity checking of the run parameter data.

Figure 3 Symbolic organization of the TSX-GEM operating system. Note that two levels of time-sharing are involved; the one ordinarily provided by TSX between process and nonprocess modes, and one between experimental users unique to this system. Note also that data reduction can take place in both process and nonprocess modes. Not shown is a provision to hold off QUEUE interrogation for ten minutes to allow jobs in the nonprocess mode to run subject only to very short interrupts for datum point acquisition.

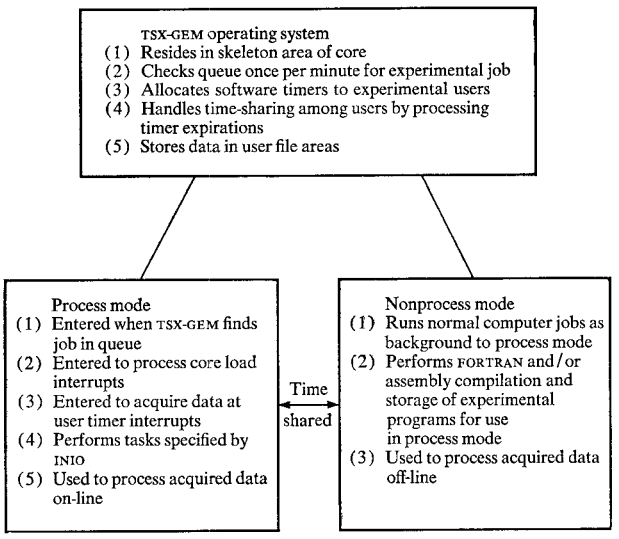
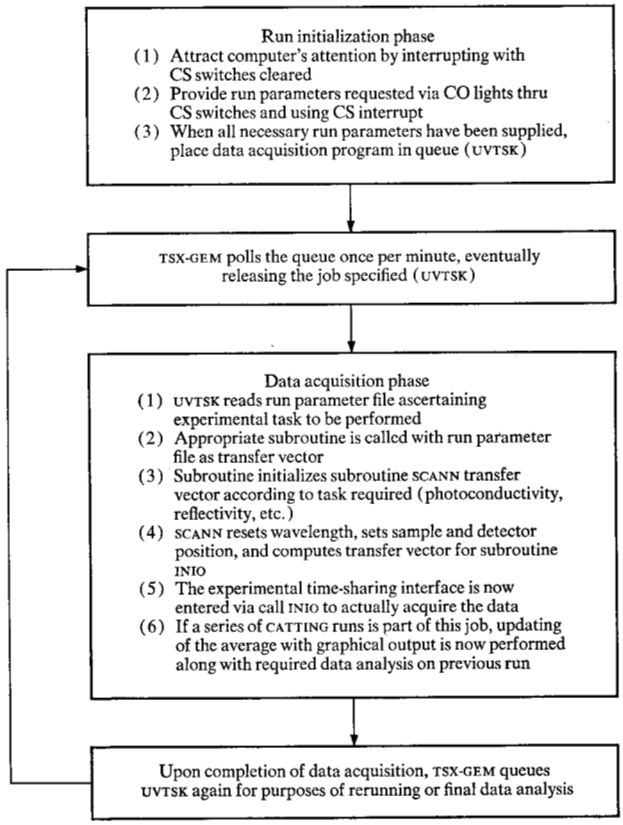


Table 4 displays what the CS switch entries might be for a typical reflectivity run. Since it is desired to perform several different kinds of optical studies using the computer, allowance has been made for up to 10 tasks. Therefore the first CS entry specifies which task, here "one" for reflectivity, is to be run. The program for our example task is called "UV1." The second entry sets up a file number for storage of the results of this run so that concatenation with other results can take place at a later time. Entries 3–6 are self-explanatory. Entry 7 specifies which resistor is to be placed in the feedback circuit of the PMT operational amplifier, the left-hand byte containing the I_0 value, the right hand, I_R. Entry 8 indicates the grating being used (see Table 1) in order that proper analysis of parameters 3 to 6 can be made. Entry 9 determines the number of times a run is repeated for the purposes of time averaging (catting). Entry A signifies the frequency of plots to be produced of the updated average on the CalComp plotter. Finally, entry B closes off the run parameter data for this operation and places the name of the data acquisition program, "UVTSK," into the TSX "QUEUE" where it resides, possibly along with other jobs, waiting to be called by TSX-GEM. Thus run initialization is over and data acquisition begins.

Table 4 Contact sense switch entries for typical UV1 run.

Contents of contact operate indicator lights (hexadecimal)	*Run parameter to be entered* (IDAT)	*Number to be placed in contact sense switches (hexadecimal)*
0001	Task to be performed (=1 for UV1)	0001
0002	ID number of disk file area where data is eventually stored (e.g., 50)	0032
0003	Initial wavelength (e.g., 6000 Å)	1770
0004	Final wavelength (e.g., 3500 Å)	ODAC
0005	Wavelength steps in 1/4 Å (e.g., 5 Å = 20)	0014
0006	Scan speed (e.g., 200 Å/min)	00C8
0007	Gain code in BCD (e.g., 17 for I_0, 24 for I_R)	1724
0008	Grating code	0002
0009	Number of times run is to be repeated (e.g., 50)	0032
000A	Interval between plots of updated average (e.g., 10)	000A
000B	End of entry mark	8000

Figure 4 This chart shows the division of the spectrophotometric experiment into two phases. The first phase relies on the 'core load interrupt' feature of TSX whereby programs residing on disk associated with a given interrupt level can be moved into core and executed upon activation of the given interrupt. Another feature of TSX that is used is the QUEUE where names of programs to be run are stored and released sequentially by TSX-GEM.



Returning to Fig. 4, TSX-GEM polls the QUEUE automatically once per minute, loading in any jobs, in order of priority, that may be found. When UVTSK is loaded and executed, it first reads the run parameter file that has just been stored. It then decides what task is to be done and branches to it via a load-on-call subroutine passing the run parameter data as an argument. All this is indicated on Fig. 6. In our example of a reflectivity run, the appropriate subroutine is UV1 shown in Fig. 7. Its main overhead job is to decide upon entry whether this run is I_0 or I_R. Assume we are about to begin the nth scan for I_0. The program, then, has just read $I_R(n-1)$ into core and has $I_0(n-1)$ available temporarily on disk. After initiating $I_0(n)$ through CALL SCANN, the ratio $R(n-1) = I_R(n-1)/I_0(n-1)$ is computed, divided by $n-1$, and

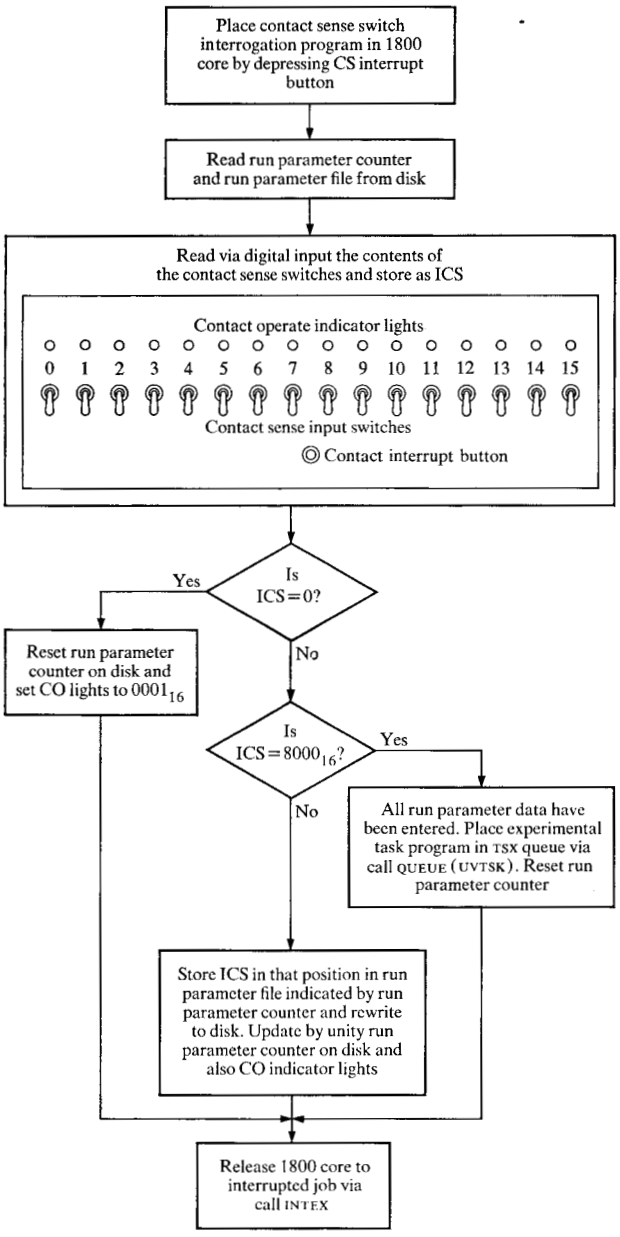
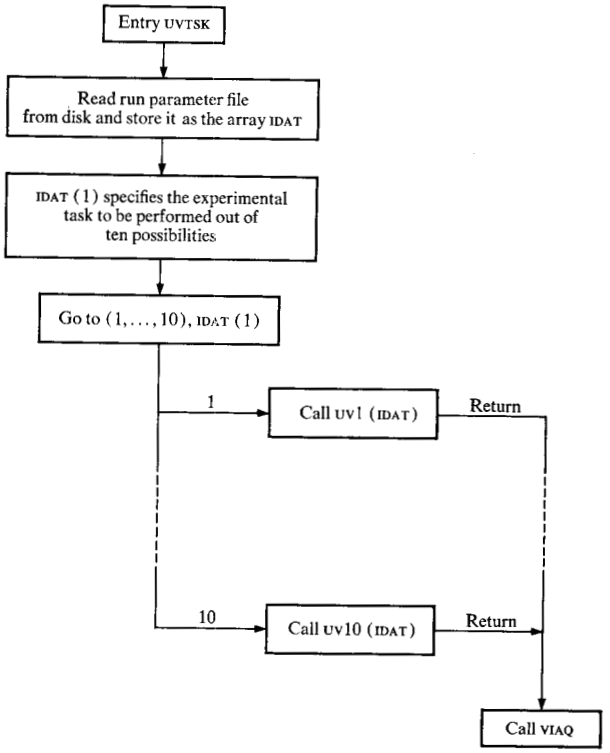


Figure 5 Flow chart of the CS switch interrogation core load interrupt program. This program is assigned to a given hardware CI level at its FORTRAN compile time and stored on disk for subsequent use. Upon activation of its assigned interrupt, it is automatically loaded into core and executed. Each ICS word forms the run parameter file that is kept on disk while the experiment is performed.

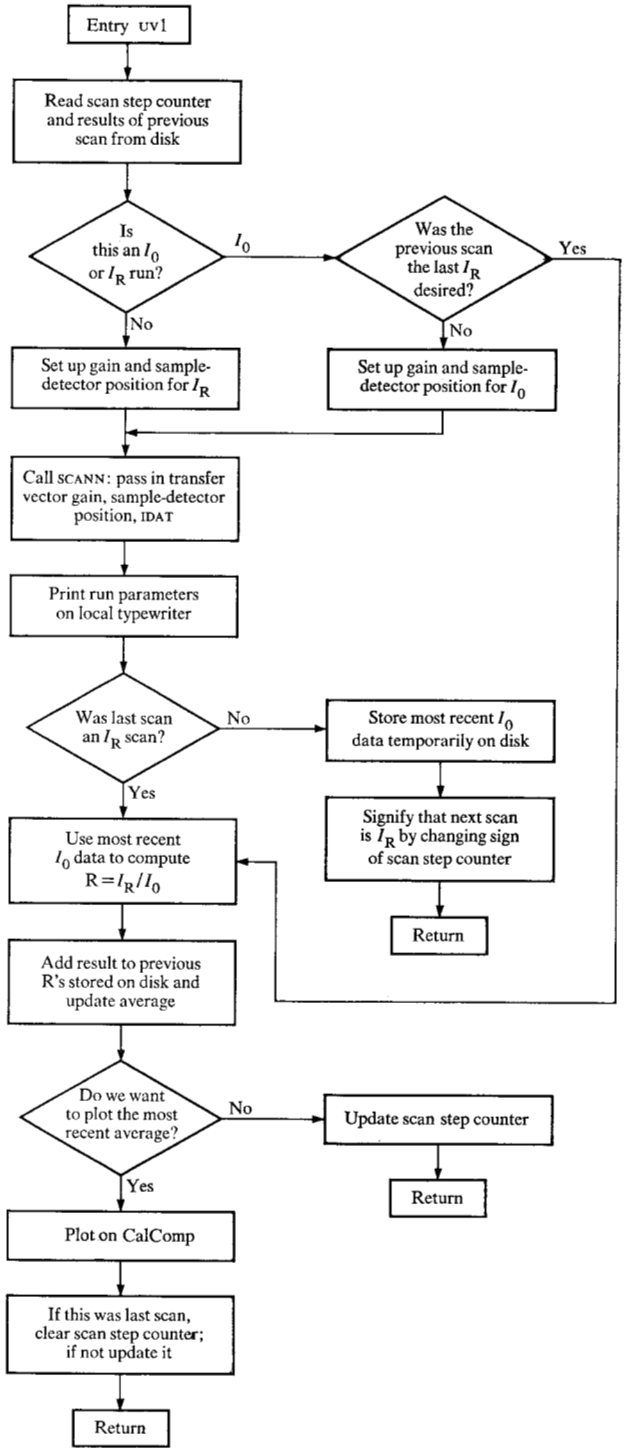
Figure 6 Flow chart of UVTSK. This program uses the first run parameter datum to select the desired subroutine for that task. In the context of Ref. 6, UVTSK is one of the EXIO routines. Each 'UV' subroutine is entered via the 'load-on-call' option which is the 1800 equivalent of the 7094 overlay procedure. In this way, the use of both core and disk storage is optimized.



added to the most recent average $\langle R(n-2)\rangle$ multiplied by $(n-2)/(n-1)$ to form $\langle R(n-1)\rangle$. Now, as will be seen shortly, one of the actions of SUBROUTINE SCANN is to queue UVTSK after the data acquisition cycle for $I_0(n)$ has been completed. Thus when UVTSK is re-entered, it determines that $I_0(n)$ was the most recent scan and that $I_R(n)$ is now to be taken, and hence deposits $I_0(n)$ on disk temporarily. Note that plots will be produced at the frequency specified in run parameter $000A_{16}$ (Table 4). That is, in the example used, 50 ratios (100 scans altogether) are to be computed and averaged and the averages at 1, 10, 20, 30, 40, and 50 are to be plotted.

Moving further into the data acquisition phase as outlined on Fig. 4, subroutine SCANN must now be discussed. This subroutine is at the heart of each UV job and its flow chart is given in Fig. 8. One of its prime tasks is to perform the bit arithmetic necessary to set up the CO words from the run parameter data. Once the electromechanical devices indicated by Figs. 2 and 8 have been initialized, the actual data are acquired through subroutine

Figure 7 Flow chart of UV1. Note that the scan step counter is incremented every other scan so that it contains the number of ratios rather than the number of scans. Whether or not a given scan is I_0 or I_R is determined by the sign of the scan step counter. Certain procedures necessary on the first entry into UV1 are not shown. Also not shown on the flow chart, but contained in the program, is a validity check of each new result against the current average. This is done to protect the current average against catastrophic equipment failure during a long "catting" run. If the rms deviation of the latest ratio from the current average exceeds a preset limit, the experiment is aborted before a new average is taken. Restart capability is provided.



INIO. The attributes of INIO, which is the experiment time-sharing software interface, is discussed in Ref. 7; here it will suffice to describe those operations it performs for our experiment. These are, for each datum taken, as follows:

(1) The contact operate bit labelled "start" in Fig. 2 is reset. When this bit is turned on, the stepping motor on the wavelength drive is incremented by the contents of the burst counter (see Ref. 6). Thus this bit must be cleared beforehand.

(2) The appropriate analog input address is read, converted, and the result stored. In our case, we use one of the low-level, double-ended, relay-multiplexed, filtered analog inputs accepting a ± 50 mV signal. We found, with proper attention paid to grounding details, almost no degradation of signal over the 300 feet of cable necessary to connect the laboratory to the computer.

(3) The "start" bit is now set and the wavelength incremented to its next position.

Thus the analog input is read *before* moving on to the next wavelength setting during each cycle. This procedure allows time for the decay of any transients that may have arisen from moving the wavelength before a reading is taken. Each cycle is repeated the required number of times at the required interval as computed by SCANN from the run parameter data. For the example provided in Table 4, the number of points read per scan would be 501 and the time interval 1.47 sec. As points are accumulated during a scan, they are placed temporarily in a disk file reserved through INIO for this experiment. It is from this file that UV1 retrieves the data after each run. After scan completion, the program UVTSK, specified in the INIO ICORE parameter, is placed in the queue. It is important to note that once INIO has initiated the scan, it performs a normal return to subroutine SCANN. Thus all subsequent operations in SCANN and UV1 take place while the experiment is under way. This is possible because all interruptions to acquire data take place at higher priority than any of the I/O operations in UV1.

The end result of a series of experiments is a set of disk files each originally designated by run parameter two (see Table 4). Each file might contain, for example, the reflectivity of a given sample over one of the wavelength regions dictated by the source-detector combination of

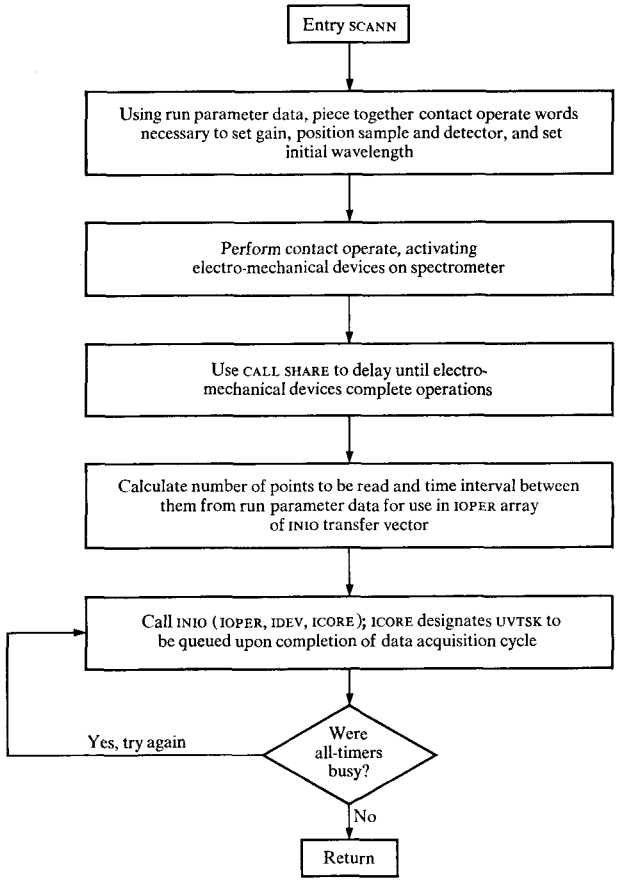


Figure 8 Flow chart of SCANN. The delay for electromechanical device reset (initial wavelength, sample-detector position) is computed from the total wavelength interval, scan rate and the fastest stepping motor speed. The time necessary to position sample and detector is much shorter than that for initial wavelength reset. The transfer vector for INIO, viz., IOPER, IDEV, and ICORE is defined in Ref. 7. It is possible that INIO will find all available timers allocated to other experiments. SCANN then keeps trying once a minute until one becomes free.

Table 2. At this point, further data reduction moves to the TSX nonprocess mode. The two principal tasks are conversion from a wavelength to an energy scale and concatenation of the different energy ranges together. The first is done through simple interpolation algorithms, while the second is attacked by trial and error because there is always some small misregistration in the overlap region between adjacent energy ranges. In addition, any necessary corrections due to source-detector drift and/or scattered light are now made. The final result is a complete spectrum as shown in Fig. 9 and a unit record copy of the data there displayed for insertion into a more suitable computer for further data reduction.

In following through the reflectivity example given in this section, the reader should not lose sight of the extreme flexibility connection of a computer to a spectrometer affords. Many problems, especially those pertaining to signal enhancement, can be effected merely by software changes instead of hardware additions. For example, to perform a differential reflectivity experiment requires ordinarily fairly sophisticated electronics and electromechanical devices. With the computer one may time average the reflectivity over many runs to improve signal/noise and then take the numerical derivative of the result.

Nor should the reader believe the approach used here is in any way unique. Although the principles underlying the application of computers to all types of scanning spectrometers are quite general, the way it is done can be as simple or as complex as one wishes. The system described in this paper evolved out of a much more elementary one. Earlier we mentioned that sample-detector control was given lowest priority in the automation scheme. That was because this feature involved extensive hardware development and the most immediate gain would result from the data logging aspect of the plan. It turned out that the latter could be implemented with alacrity and was carried out in the following way:

(1) The CS switch and CO indicator light panel shown in Fig. 5 were constructed and connected to the computer. Also, the recorder output of the phase-sensitive detector was wired to an 1800 ADC input. In addition, the sign bit of the CO indicator lights was made to operate a relay which turned on the McPherson-supplied wavelength drive synchronous motor. This completed the initial hardware required.

(2) Run parameter data were supplied in much the same way as described above. However, the operation of the scan was completely different. INIO has a feature whereby a CO group can be initialized to a desired value and then updated by a given constant as each analog-to-digital read is performed. Thus the CO indicator lights were set to the two's complement of the number of points to be taken, thereby turning on the sign bit and the synchronous motor, and were increased by one on reading each datum. On the last point read, the CO group cleared, therefore turning off the motor. Because of the highly accurate, and known, speed of the synchronous motor, all that was additionally needed was to record the time, relative to turning on the motor, that each point was read. This was accomplished through another feature of INIO which allowed the reading of one of the computer internal clocks concurrently with analog-to-digital conversion. Thus, a table of phase-sensitive detector readings vs. time intervals was built up during each scan.

(3) Nonprocess software was created to handle interpolation and convert time intervals to wavelength and energy intervals via the constant synchronous motor speed. Sample-detector manipulation and wavelength resetting were done manually to initiate I_0 and I_R scans which were

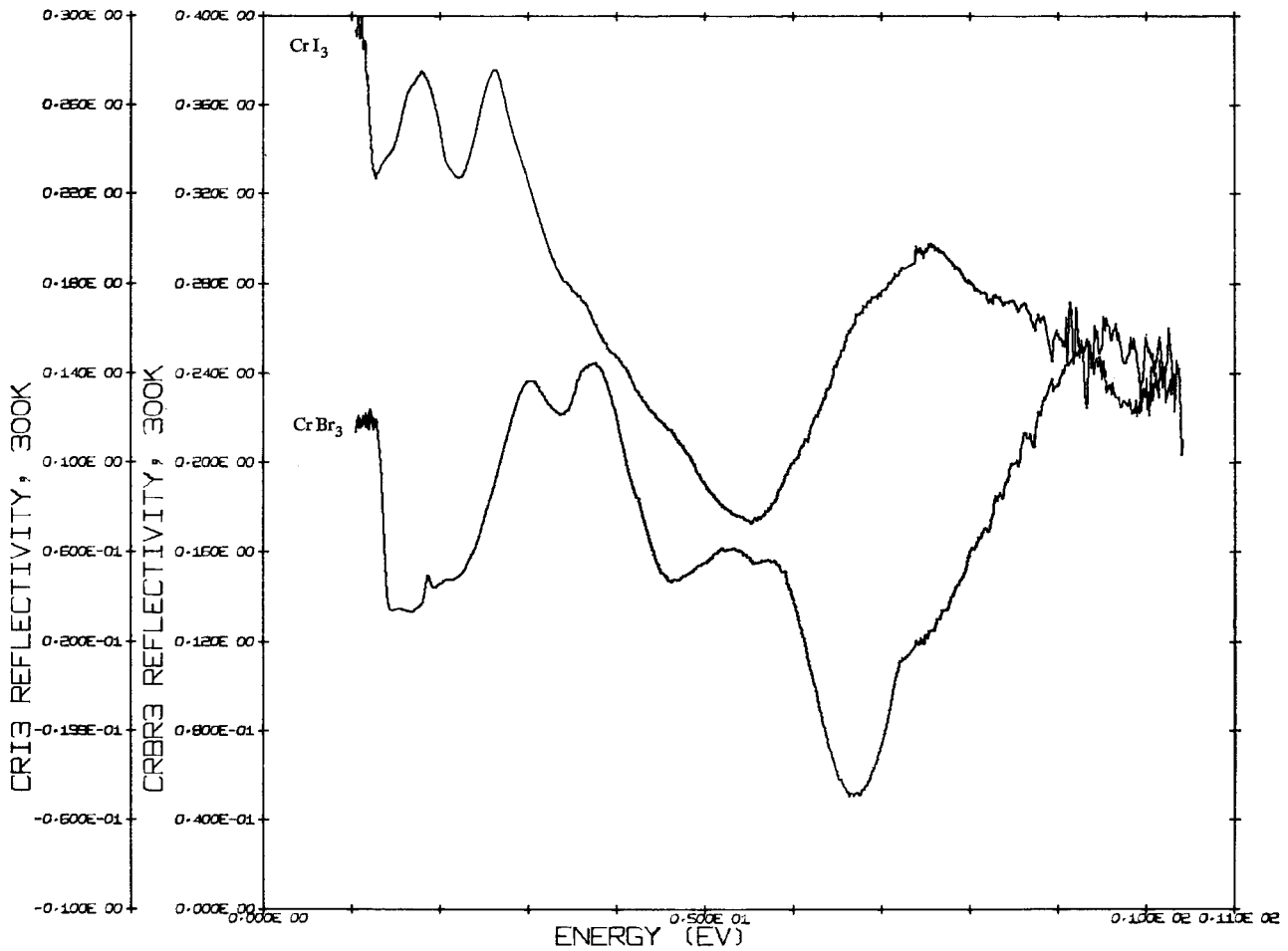


Figure 9 Reflectivity spectrum of $CrBr_3$ and CrI_3 at room temperature. Because it was our intention not to let the automation implementation unduly interfere with experimental progress, data in different portions of the spectrum were taken with the system in different stages of evolvement. As mentioned in the text, measurements in the range 8 to 10.5 eV were made under the free-running system, whereas those at other energies were taken under computer control of the wavelength setting.

then subsequently stored. Off-line data processing then produced the ratios and did time averaging if sufficient runs were available.

It turned out to be possible to implement the above operation in about 15 man-days and it accrued to us most of the advantages of the more advanced system now in existence. A major fault of the early system was that interpolation introduced small amounts of jitter which had the effect of producing small mismatches in energy between I_0 and I_R scans. This was unimportant at longer wavelengths where spectral sources are more or less continuous, but in those regions where hydrogen lines are used, misalignment noise occurred in the ratio. This can be seen in the 8 to 10 eV range of Fig. 9. Nonetheless, the simplicity of the method recommends it for application to other experiments. It seems possible, for example, that this approach could provide a quick and easy data logging capability for such instruments as IR spectrometers, vapor phase chromatographs, and scanning x-ray and magnetic resonance spectrometers. There are, however, some experiments (perhaps mass spectroscopy) which require complete dedication of the computer for a given period of time that, if long enough, could cause significant data loss to one of these free-running operations. If such interruptions were no longer than a few seconds in length, however, this loss would not be serious and could be made up through interpolation. Of course, those experiments whose independent variable was under the control of the computer via a stepping device would not suffer at all.

We should mention that the scheme of having a single coreload (UVTSK) assign the data acquisition tasks via load-on-call (LOCAL) subroutines is not unique. The same end could have been accomplished through queueing

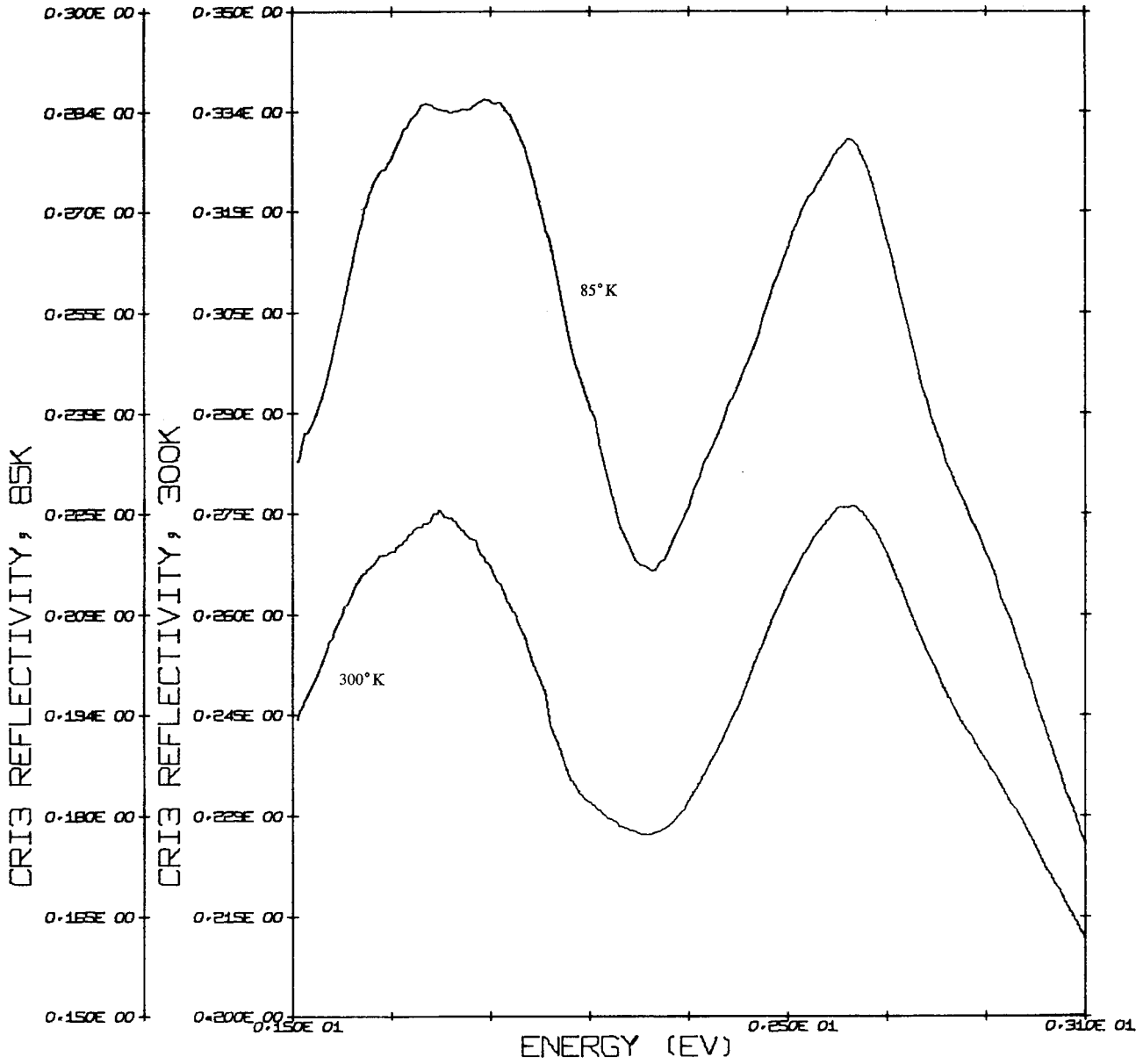


Figure 10 Low-temperature behavior of the two low-energy reflectivity peaks in CrI_3.

different data acquisition core loads from the CS switch interrogation interrupt core load or by using the CALL SPECL option of TSX from UVTSK. Both methods, however, require complete core loads to be built for each data acquisition job, whereas the load-on-call feature just brings in the bare 'un-link-edited' subroutine from disk which then picks up its own requisite subroutines from those already in core. In this way, the use of both core and disk space is optimized.

Conclusions

It is natural that we should now discuss some of our experimental results in light of the aims stated in the Introduction. Figures 9 and 10 show the reflectivity spectrum of two magnetic insulators, $CrBr_3$ and CrI_3; Fig. 9 in particular shows the raw ratio over the energy range 1 to 10.5 eV. In view of these data, let us then take up each of the three original points one-by-one.

(1) The double-scan method was used to gather data

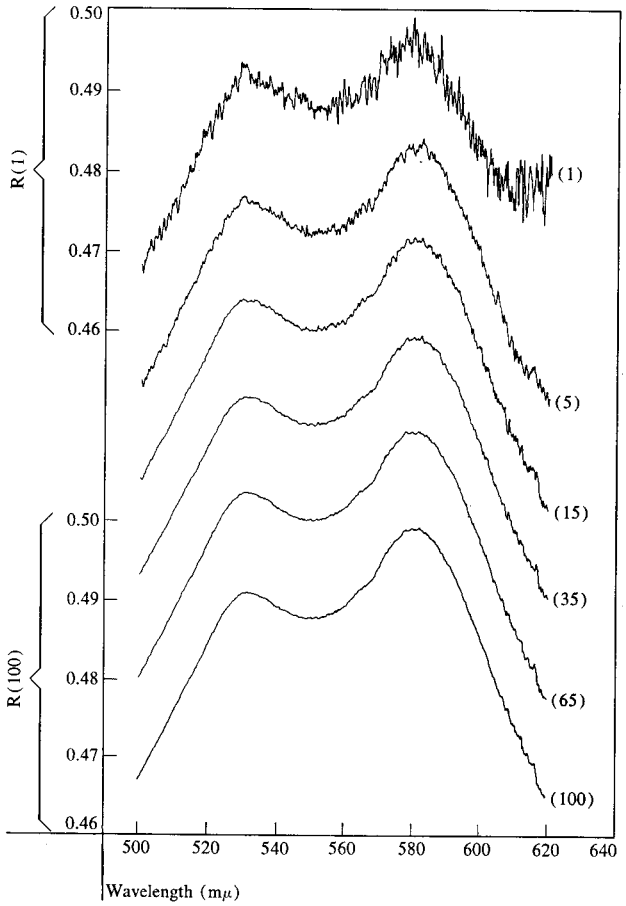


Figure 11 Reflectivity spectrum of the germanium Λ spin-orbit doublet. This figure represents the average of up to 100 scans at signal/noise intervals of approximately 2, 4, 6, 8, and 10. The total number of equally spaced points per scan is 601. All curves are plotted to the same scale, but only those for the first and one-hundreth are shown in proper perspective. The amplitude resolution is judged to be about 0.001 and does not necessarily represent an ultimate figure.

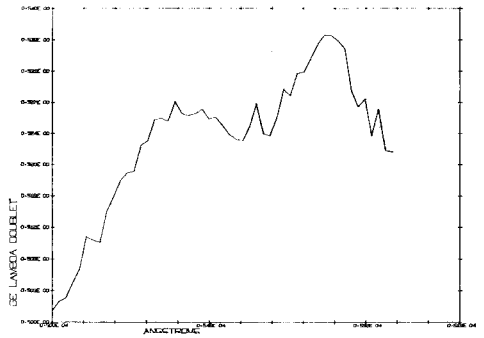


Figure 12 Reflectivity spectrum of the germanium Λ doublet as found by computing the ratio manually. The scale is the same as Fig. 11 and the data were taken from Ref. 10. The number of equally spaced points is 51.

for ratio computation. The computer completely eliminated the manual transcriptions and calculations previously involved in this mode of operation.

(2) The results presented in Fig. 9 represent the concatenation of measurements over six different energy ranges. This was effected by manipulating the data entirely within the computer in the manner described in the previous section. Figure 9 is the graphical output of the computer on completion of this task. Furthermore, the data exists in storage in much finer detail than shown on Fig. 9. We have the capability of "blowing-up" and presenting in graphical form interesting detail. Figure 10 demonstrates this for the low-temperature behavior of the two low-energy peaks in CrI_3.

Inasmuch as the data necessary for the production of Fig. 9 is retained in computer storage, it is a trivial matter for these to be reproduced in unit record form for insertion into a more powerful computer.

(3) The spectra presented in Fig. 9, especially at lower energies, possess a quality higher than that of the usual reflectivity measurements, because they are derived from the average of at least two, and sometimes five, repetitive scans. Those familiar with reflectivity spectra will recognize in Fig. 10 the uniqueness of such data with so low a noise level over a four-percent spread in amplitude.*

In order to further demonstrate the efficacy of time averaging by repetitive scans, a *tour de force* experiment was performed on the well-known and intensively studied Λ spin-orbit doublet of germanium.[9] The results are shown in Fig. 11. The initial noise level is fairly high because a very small spectral slit width and short *RC* time constant were used. Each ratio scan took about five minutes, the total 100 repetitions requiring approximately 9 hours during which the apparatus was completely unattended. Note that by scan 15 all significant structure is apparent and that further averaging results only in minor smoothing. This is, of course, because the greatest improvement in signal/noise occurs during the early scans due to the $\sqrt{n}$ rule. In actual practice, the experiment would have been terminated between scans 5 and 15 and an appropriate digital filter then applied for smoothing purposes.

The improvement in amplitude resolution over that obtained by manually ratioing I_0 and I_R scans arises primarily from the extra significant figure recorded by the 1800 analog-to-digital converter. That is, when one visually transcribes data from a strip chart recorder for a later ratio computation, one usually attains only three significant figures whereas the 1800 ADC will record

* It is not within the scope (nor was it the intent) of the present paper to discuss the physics of these data. This will be done in a later publication.

approximately four. An illustration of the difference this makes is afforded by Fig. 12, which is a plot on the same scale as that of Fig. 11 of data taken and reduced manually.

We believe some of the more exciting applications of our system will be to the various modulated optical response experiments (electroreflectivity, piezoreflectivity, etc.). The noise level of these measurements is usually quite high, engendering the hope that the time-averaging capability of the computer-assisted spectrometer aided by digital filtering and structure enhancement procedures can drastically reduce it.

A final word is in order concerning the impact of on-line computer capability on the manner in which our experiments are now performed. Generally, one goal of an experimental solid state physicist should be to keep his equipment in as flexible a state as possible to insure rapid implementation of new measurement ideas or techniques. Unless one is careful, the introduction of a computer into the apparatus can retard this flexibility, especially if a complicated hardware interface is employed. The author, from his own experience, has found that keeping the interface as simple as possible and concentrating on software construction to respond to new experimental situations has actually enhanced flexibility. Once the requisite skills have been acquired, it is far easier and more rapid to "re-wire" the experimental apparatus through programming than by re-configuring hardware.

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