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The construction of a single crystal neutron diffraction unit and measurement of effective neutron temperature

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THE CONSTRUCTION OF A SINGLE CRYSTAL NEUTRON DIFFRACTION UNIT AND MEASUREMENT OF EFFECTIVE NEUTRON TEMPERATURE

by

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A

THESIS

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ABSTRACT

The continued expansion of the nuclear reactor facility and the nuclear engineering program makes it desirable that a neutron spectrometer be available at the reactor facility. This unit would be available for use in graduate and undergraduate laboratories and for graduate research.

A single crystal, white radiation spectrometer including collimator, automatic controls, and shielding was designed and constructed.

The performance of the unit was checked using LiF and Cu crystals. A rocking crystal curve and a $\theta - 2\theta$ curve was obtained with each crystal. The effective neutron temperature was then determined from the LiF crystal $\theta - 2\theta$ curve.

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I. INTRODUCTION AND LITERATURE REVIEW

Elsasser[1] first suggested in 1936 that the motion of neutrons could be determined by wave mechanics, and therefore, they could be diffracted by crystalline materials. The diffraction of x-rays had already been verified by Von Laue in 1912. Experimental demonstration of neutron diffraction was performed by Halban and Preiswerk (1936) and by Mitchell and Powers (1936). These experiments used radium-beryllium sources which did not produce monoenergetic neutrons. The neutron intensity was also low. Neutron diffraction became of real interest with the advent of nuclear reactors which provided a source of neutrons of sufficient intensity to make detailed studies possible.

The first true neutron spectrometer or diffractometer was constructed by Zinn at Argonne National Laboratories in 1945[17].

The diffraction of x-rays and neutrons in a crystal can be described by Bragg's equation[16]

$$n\lambda = 2d \sin \theta$$

where $n\lambda$ is some integral multiple of the wavelength λ, d is the interplaner spacing and θ is the angle of incidence of the beam onto the crystal. Coherent reflection occurs only when this equation is satisfied. Non-coherent scattering also occurs, but the intensity is usually far below that of the coherent beam. Normally n is taken as one and higher order reflections would be considered undesirable interference. Since the reflected beam leaves the crystal at an angle equal to the angle of incidence, it can be seen that if the crystal rotates through an angle θ that the reflected beam will rotate through an angle 2θ with respect to the incident beam.

Neutrons have two advantages over x-rays in diffraction studies. These advantages are that neutrons will penetrate further into heavy element materials and neutrons can be used to easily determine the location of light atoms in a crystal lattice[1]. The second advantage is due to the fact that the scattering cross section is relatively independent of the atomic number.

Much of the neutron diffraction work being done today involves the detailed study of crystal structure. This type of work requires a monoenergetic source of neutrons. However, the neutrons coming from a reactor are not monoenergetic but have an energy distribution described by the Maxwell-Boltzmann equation[4]

$$\frac{n(E)}{n} = \frac{2}{(\pi KT)^{3/2}} \epsilon^{-\frac{E}{KT}} E^{1/2}$$

where n equals the number of neutrons, K equals the Boltzmann's constant (1.380×10^{-23} joules/molecule - °K), T equals the temperature (°K), and E is the energy of the neutrons (Mev).

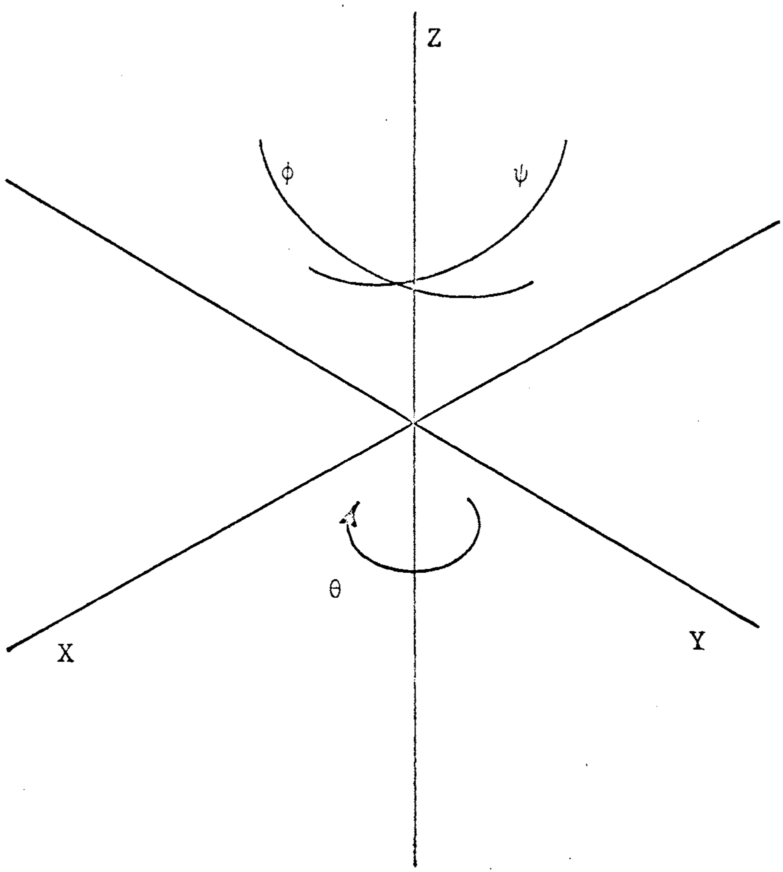
One of the common methods of obtaining a monoenergetic beam of neutrons is to use one crystal (generally lead, or beryllium) as a monochromator. The wavelength of the neutrons reflected at an angle θ from the crystal or an angle 2θ from the primary beam is determined by using the Bragg equation. The sample to be studied is then placed in the secondary beam, that is, the beam of neutrons reflected from the monochromator crystal. The energy of the beam striking the sample can be changed simply by changing the angle between the sample and the primary beam.

If, however, only one crystal is used, the number of neutrons reflected at some angle θ should be proportional to the number of neutrons with a wave length satisfying the Bragg equation for that angle. Using this fact, the neutron spectrum can be measured[8]. The results should follow the Maxwell-Boltzmann distribution. The effective neutron temperature, which is generally 50 - 150°C above the moderator temperature, can be determined by applying the Maxwell-Boltzmann equation to the spectrum obtained experimentally[18].

General Design Features: To define the beam direction, a collimator is placed in the primary neutron beam; this limits the divergence, or angular spread of the beam from the axis of the beam. The design of this collimator varies with the type of experiments to be performed. For accurate resonance analysis the horizontal angular divergence of the neutron beam should be on the order of one or two minutes of arc[14]. Many other neutron diffraction experiments including reactor spectrum measurements make a coarser collimation desirable. A divergence of about 10 minutes of arc is a good compromise for a universal collimator[8].

One common method for obtaining good collimation while maintaining a reasonable sized opening is to use a number of parallel channels. This type of collimator is called a Soller Collimator. Collimators of this type were first used in x-ray work.

In general it is desirable that some sort of adjustable crystal positioning device or goniometer be used. This goniometer should have two axes of horizontal position denoted x and y, so that the crystal can be accurately centered over the axis of rotation. Also, two axes of rotation phi (ϕ) and chi (χ) should be available for proper orientation of the crystal planes. The center of rotation for these two axes should be the center of the crystal face. These axes of rotation are shown in Figure 1.



Axes of Motion

Figure 1

Two types of detectors are in general use in neutron diffraction. These are boron triflouride (BF_3) proportional counters and fission counters. The BF_3 counters normally use a high enrichment (~95%) of B^{10} and operate at a gas pressure of 40 to 70 cm Hg. Although boron has an approximate $\frac{1}{v}$ reaction cross section, the counters are designed so that they are essentially black to thermal neutrons; therefore, the sensitivity is nearly constant. The fission counters use highly enriched (90%+) U^{235} as the fissioning material. The sensitivity would vary as the fission cross section of U^{235} which is not $\frac{1}{v}$.

The shielding around a neutron diffraction experiment must comply with Title 10 Part 20 of the United States Atomic Energy Commission regulations. In general the radiation level in an area open to normal access must be less than 2.5 mr/hr.

Shielding is generally much more of a problem with a single crystal unit than for the double crystal unit. In a double crystal unit the monochromator crystal can be mounted in a large stationary shield with a small slot to extract a neutron beam for the second crystal. The primary neutron beam and the gamma beam from the core are attenuated by the stationary shield. The only other shielding needed is a beam catcher behind the second crystal to attenuate the secondary neutron beam. There are essentially no gamma rays outside the stationary shield. However, in the case of a single crystal diffraction unit, the crystal must be in the primary beam from the reactor. The crystal cannot be mounted in a stationary shield and a slot used as in the case of a monochromator since a large scan angle is necessary. The neutrons can easily be stopped with a beam catcher, but the gamma rays present a problem. One solution to this problem is to place a lead plug in front of the collimator. However, incoherent scattering of the neutron beam will occur in the lead[8]. The maximum thickness of lead that can be used is limited by the fact that only a certain amount of scattering can be tolerated. The University of Maryland Reactor (10 kw, pool type) is using a single crystal unit with no gamma shielding in the primary beam in front of the crystal[2]. A 16-inch-thick lead beam stop serves to attenuate both neutrons and gammas; this is placed behind the diffraction unit. The Livermore Pool Type Reactor (2 Mw) uses a 6-inch-thick lead plug at the front of the beam tube[8]. The diffraction unit is enclosed with a 4-inch-lead wall in the path of the gamma beam. Water tanks are placed around the unit to provide additional shielding.

A beam catcher can be constructed from borated paraffin. At least 0.3 pounds of boric acid per pound of paraffin should be used in the region where the beam strikes the paraffin. The advantage to borated paraffin over, say, cadmium and paraffin laminated is that no capture gamma rays are emitted when boron absorbs a neutron. In addition, a borated paraffin beam catcher is cheap and easy to construct.

The detector shield, which can also be constructed of borated paraffin, normally serves as a beam catcher for the reflected neutrons. The shield also serves to shield the detector from neutrons other than the reflected beam. This often requires more shielding than would be required to attenuate the secondary beam.

It has been previously stated that as the crystal rotates through an angle θ, the reflected beam rotates through an angle 2θ. From this fact, some form of coupling with a 2:1 ratio between the detector arm and the crystal table is desirable. Two types of coupling can be used, mechanical or electrical. Mechanical coupling can be achieved through the use of gears[11] or the use of steel tapes riding over steel drums[8,13,6]. The electrical coupling uses a separate pulsed stepping motor to drive the crystal table and the detector[10,5]. A 2:1 ratio is obtained by the use of a multivibrator to obtain a 2:1 pulse ratio. Electrical coupling readily lends itself to automatic operation.

Description of Equipment in Use at Other Facilities: The new double crystal at Argonne's CP-5 reactor uses three interchangeable Soller Collimators with horizontal divergences of 21.2 minutes, 27.7 minutes, and 58.8 minutes[10]. These have openings of 0.756 x 1.874 inches, 0.599 x 1.741 inches and 0.393 x 0.393 inches, respectively.

Some work has been done using coated channels in a Soller Collimator in an attempt to reduce reflection from the walls. Cadmium coatings on the surface of the channel walls have very little effect[7]. Tetradecanoic acid ($C_{14}H_{28}O_2$), also known as myristic acid, has been found to provide excellent reflection suppression. A 2 mil thickness will completely mask the reflection properties of the base material.

The Harwell BEPO single crystal spectrometer unit uses a collimator consisting of 14 strips of steel 0.022 inches thick and 59 inches long separated by 0.088 inches thick steel spacers[13]. The final aperture is 1.6 inches square.

The University of Maryland Reactor uses lead blocks with an opening cut through the blocks as a collimator[2]. The single channel measures 1/2 inches horizontal by 2 inches vertical.

The diffraction unit at the Livermore pool type reactor provides the 4 axes of motion, previously described, plus rotation about the vertical axis for crystal angle alignment[3,8]. Electric motors are used to drive the three rotational motions. Remote readout of position is obtained by use of syncho-torque transmitters and receivers which are used to operate Veeder-Root registers. The Livermore group calls their crystal positioning device an Eulerian cradle.

Two different positioning devices are in use on the large diffraction units at Argonne National Laboratory. One is a universal goniometer which provides motion in the x, y, ϕ, and χ directions[11,8]. This goniometer is capable of supporting a load in excess of 100 pounds. It was designed to support cryostats or furnaces as desired.

The second type is the full circle goniostat[12]. This unit provides full circle rotation in the ϕ direction plus provisions are made to rotate the crystal about its axis in the plane of the ϕ rotation.

Several neutron diffraction units now in use have been set up for automatic operation. Included in these automatic units are the large diffractometers at Argonne National Laboratory[10,11], the BEPO unit[13], and a unit at Kjeller, Norway[15].

In general these units are programmed to take a count at one angle setting, print out or store in a memory the angle setting and counts, rotate to a new angle and then repeat the process. In some cases, more than one sample is studied at a given angle. The samples can be changed automatically; then after the series of samples has been run, the unit rotates to a new angle then repeats the process.

The latest unit in operation at Argonne National Laboratory uses a punched paper programming tape to control the sequence of operations. This gives the unit great flexibility.

<u>Data Obtainable with Single Crystal Diffractometers</u>: The neutron energy distribution can be described by the Maxwell-Boltzmann equation as previously discussed. The so called "white radiation" which is

used with a single crystal diffraction unit should follow a Maxwell-Boltzmann distribution.

Normally, two types of curves are obtained with a single crystal unit. The first is a rocking crystal curve which is taken with the detector fixed at some angle. A series of counts is then made as the crystal is rotated through the angle which gives peak counts from the detector. If the detector is fixed at an angle of 2α then the peak will occur when the crystal is at an angle of α.

Sailor, et al,[14] has shown that the rocking crystal curve in a beam of white radiation can be approximated by a normal distribution with a standard deviation.

$$\sigma = \left(\frac{W^2}{2} + \eta^2 \right)^{1/2}$$

for the distribution

$$J(E) = J(0) \exp - \frac{E^2}{2\sigma^2}$$

and

$$\eta = \frac{b}{2\sqrt{2\ln 2}} \qquad W = \frac{a}{2\sqrt{2\ln 2}}$$

where J(E) is the probability of finding a mosaic block with a tilt between E and E + dE, J(0) is the normalization constant, b is the mosaic spread of the crystal, and a is the horizontal angular divergence of the neutron collimator.

For a normal distribution the full width at half maximum equals β where

$$\beta = 2\sigma\sqrt{2\ln 2}$$

From the above and the fact that the horizontal angular divergence of the collimator can be calculated, the mosaic spread of the crystal can be evaluated.

The second type of curve which is normally obtained is a $\theta - 2\theta$ curve. A $\theta - 2\theta$ curve yields a neutron spectrum which should follow the Maxwell-Boltzmann distribution fairly closely. The curve can be corrected for background by running a second curve $(\theta + \Delta) - 2\theta$; where Δ is some angle just large enough to place the detector out of the refracted beam. This angle can be determined from the rocking crystal curve. The angle would be that angle just beyond where the peak joins the background region. The counts obtained would be subtracted from the counts obtained at corresponding 2θ angles of a $\theta - 2\theta$ curve. This approximately corrects for normal background and non-coherent scattering from the crystal.

The energy corresponding to the peak in the $\theta - 2\theta$ spectrum is the most probable energy. By using the Maxwell-Boltzmann relationship the effective neutron temperature can be calculated[8].

Advantages and Disadvantages of a Single Crystal Diffractometer: The equipment for a single crystal diffractometer is somewhat simpler than that for a double crystal unit since only one crystal table is involved. In most cases, however, the first table of a double crystal unit is operated manually so that the automatic equipment would essentially be the same for a single or double crystal unit. A single crystal diffractometer can be made very simple if desired; an example of this is the one used at the Argonaut Reactor at Argonne National Laboratory[18].

The two largest problems with a single crystal diffractometer are shielding, which has been discussed, and the interpretation of data. If experiments other than rocking crystal curves and spectrum measurements are attempted, the interpretation of data becomes very difficult since the incident beam is a continuous spectrum.

Present Work: The object of the work described in this thesis was to design, construct, and perform initial tests on a single crystal neutron diffractometer to be used at the University of Missouri at Rolla Reactor Facility. The purpose of constructing the unit was to provide a neutron diffractometer which could be used for graduate research, undergraduate and graduate laboratory experiments and which could be used to measure the reactor thermal neutron spectrum. This would provide the first measurements of the thermal neutron spectrum of the reactor.

The equipment was designed to be simple to operate, yet be adequate for accurate research work. The equipment was also designed for fully automatic operation.

Initial tests were performed using lithium flouride and copper crystals to obtain rocking crystal curves and θ - 2θ curves.

II. EXPERIMENTAL PROCEDURE

A double crystal neutron diffractometer yields much more useful information than a single crystal unit. However, it was decided that the unit to be constructed would be a single crystal diffractometer since the neutron flux in the beam tube (10^8 n/cm^2/sec) is not sufficient for double crystal diffraction studies. The present unit is designed so that it can easily be modified for use as the second crystal table in a two crystal unit. The following are some of the criteria used for the design of the single crystal diffraction unit.

1. The unit should be as versatile as possible. It should be simple enough for use in laboratory experiments yet be suitable for use in graduate research.
2. The unit should be rigidly constructed. The crystal table and goniometer should be capable of supporting a furnace, a cryostat, or small magnets. A load of 100 pounds was selected as the design load.
3. If possible, the unit should be designed for automatic operation.
4. Adequate shielding must be provided. A neutron beam catcher must be provided and some means must be provided to attenuate the gamma beam. Access to the areas in the region of the primary and secondary neutron beams must be restricted. Some means must be provided to warn personnel that the beam port is open and that the area is hazardous.
5. The collimator to be used with the unit should also be as versatile as possible. Some means of closing the collimator port while the reactor is at power is desirable. This would allow changes to

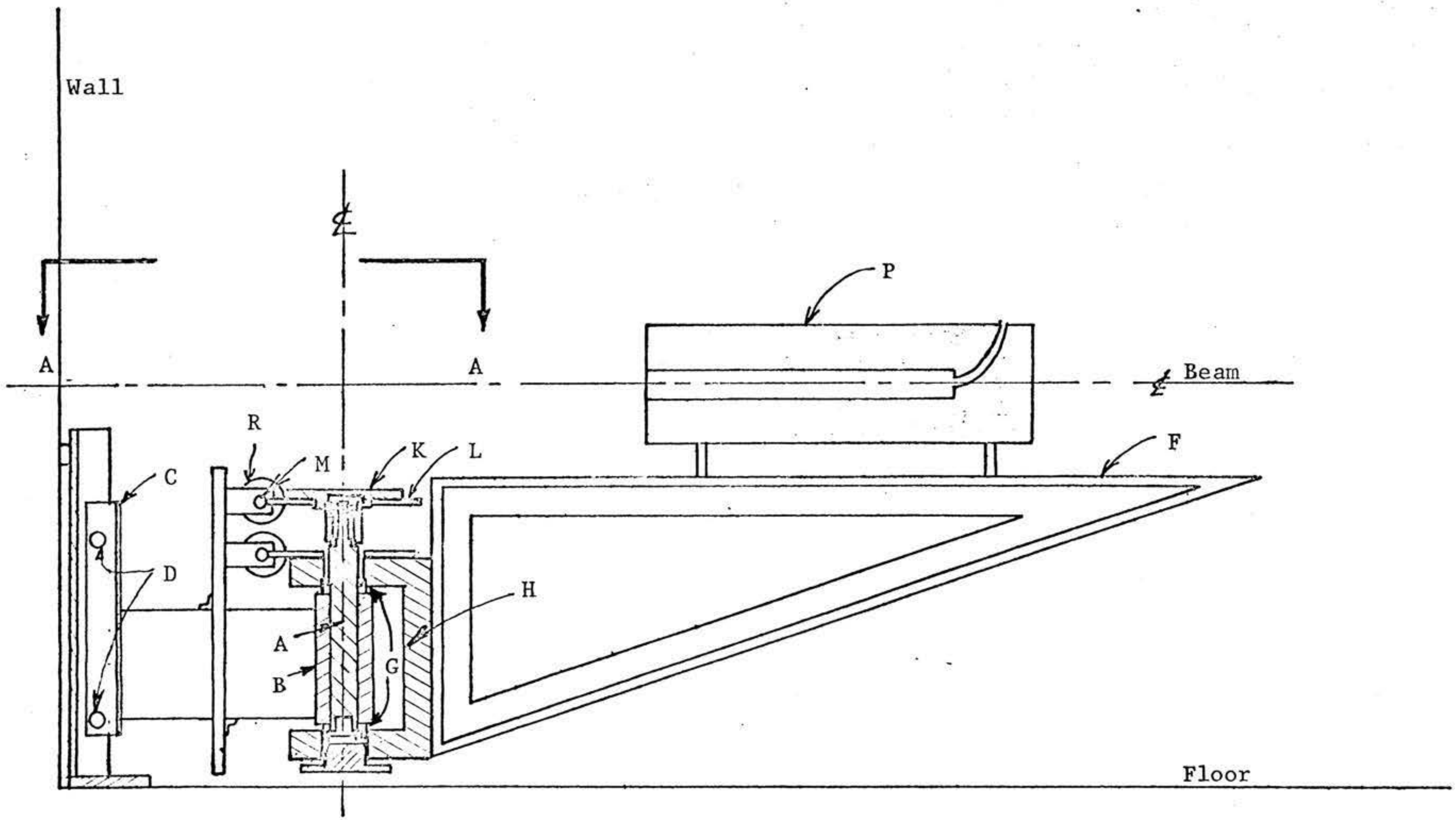
be made on the unit while the reactor is at power. The collimator port, when closed, should reduce the radiation level to less than 2.5 millirem per hour in the work area.

6. The detector should be suitable for neutron diffraction work. It should preferably be black to low energy neutrons traveling parallel to the axis of the counter.

Some rather severe restrictions were placed on the design by the height of the centerline of the beam port above the floor. The funds available for construction were also limited.

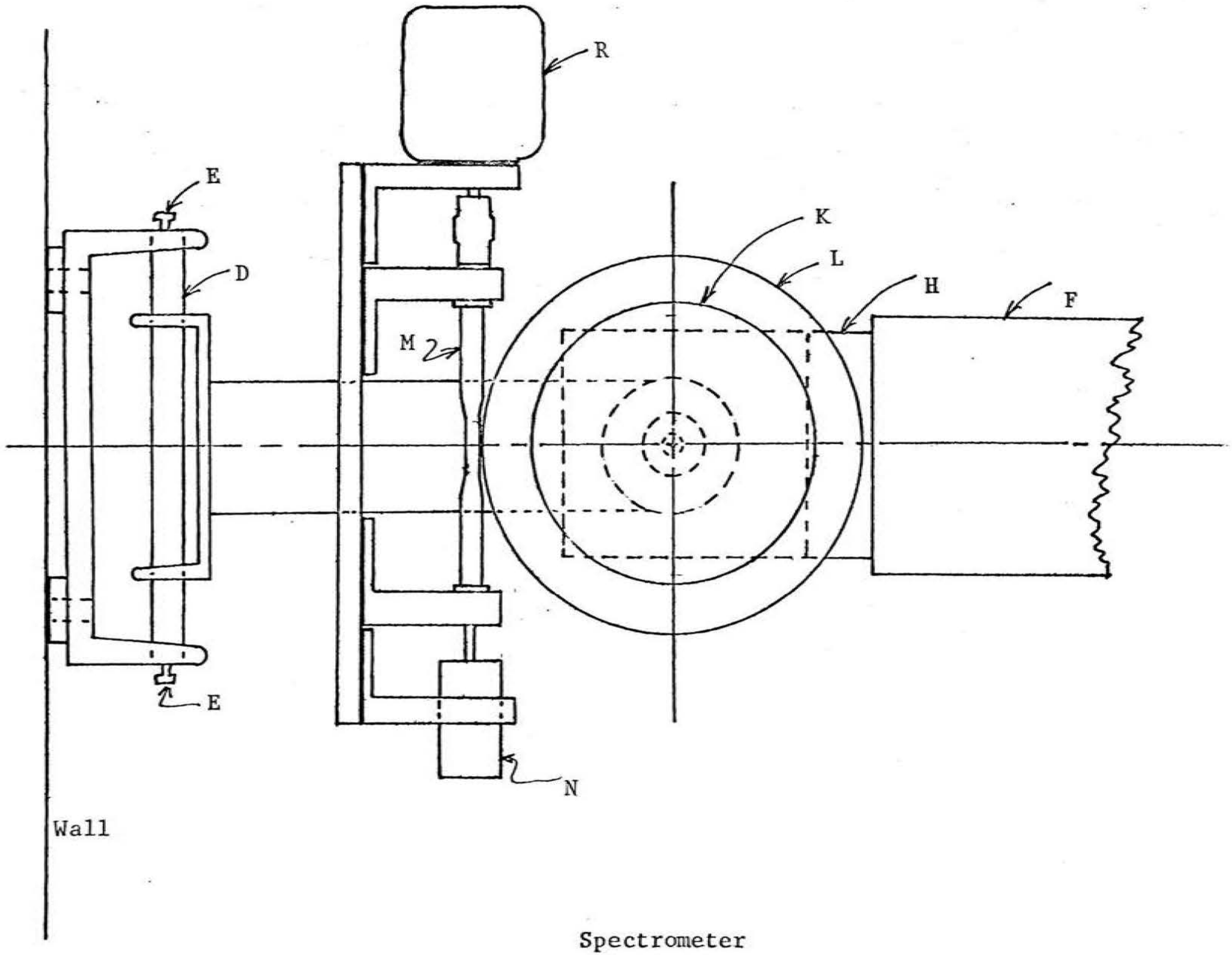
The design of the neutron diffractometer follows the design of the $\Delta\lambda$ portion of Argonne National Laboratory's Spectrometer II as described by M. H. Mueller, et. al.[11]. The unit is shown in Figures 2, 3, 4, and 5. The unit is essentially an axle A, which passes through a metal cylinder B. The cylinder is supported by a steel I-beam which is welded to the wall assembly which in turn bolts to the beam tube face and a base plate which is anchored to the floor. The wall assembly consists of a movable portion C, which rides on two bars D. Four bolts E, are used to adjust the position. This allows the axis to be centered in the beam and allows slight rotation of the axis in a plane parallel to the wall which allows the axis to be adjusted to vertical in one plane. Vertical adjustment in the second plane can only be obtained by adding or removing shims from between the fixed portion of the wall assembly and the beam tube face.

The detector arm, F, is bolted to a large steel "U", H, which is supported from the axle by two sets of Timken angular contact bearings, G. These bearings are designed to support an axial load as well as a radial load. The tension on the bearing is adjustable. The crystal table, K,



Cross Section of Spectrometer

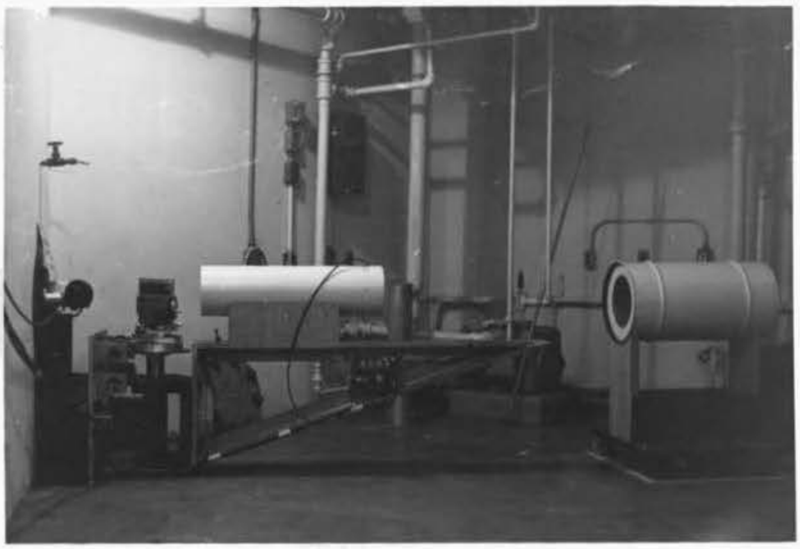
Figure 2



Spectrometer

Section AA

Figure 3



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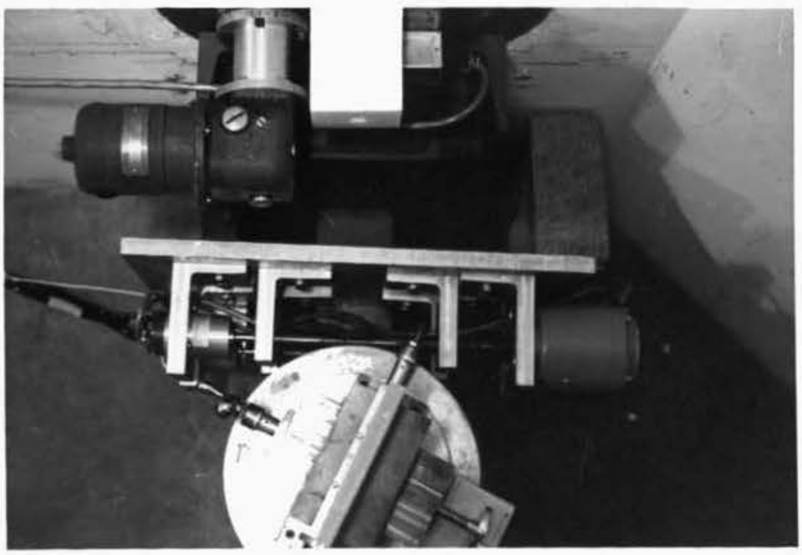
Side View of Unit

Figure 4



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Top View of Drive Unit

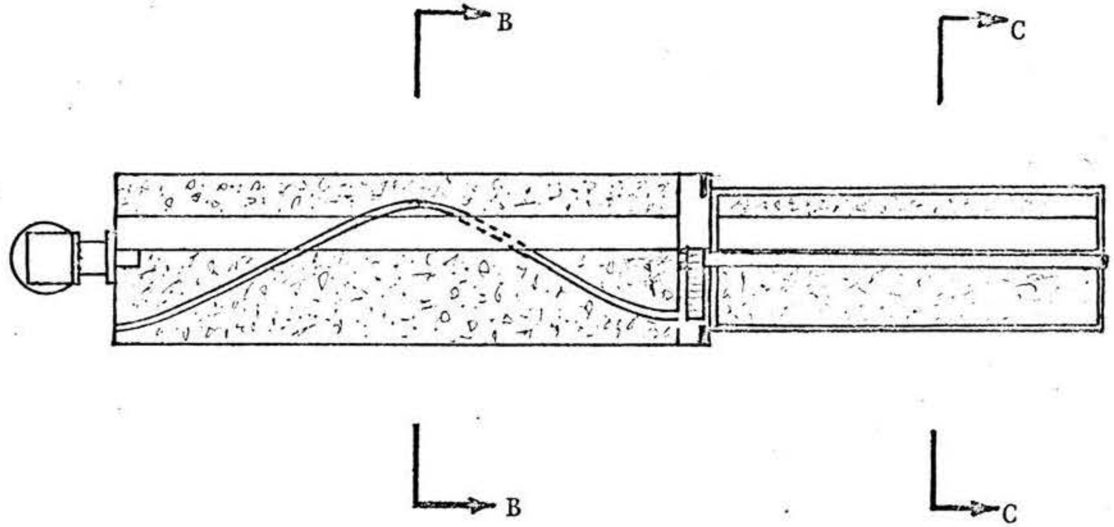
Figure 5

is also supported by Timken angular contact bearings. A 360 tooth worm gear, L, is attached to the crystal table, K, and to the "U", H. The drive gears, M, are each supported by two Timken angular contact bearings and are coupled to a Superior Electric SS-250 pulse motor, M. A selsyn generator, N, is attached to each drive gear to provide remote angle readout. A 360 tooth gear was used to give a ratio such that one rotation of the drive gear gives one degree of rotation of the detector arm or crystal table. Selsyns provide remote angle readout to ± 0.03 degree.

The detector, a Reuter Stokes #RSN-108S-MG BF_3 proportional counter is housed in a borated paraffin shield, P. The shield has about 0.3 pound boric acid per pound of paraffin. A minimum of 3 inches is provided in the walls and a minimum of 5 inches is provided behind the detector.

The design of the collimator, Figures 6 and 7, follows no known design directly. A 1 3/4 inch by 2 3/4 inch opening is provided through the two sections. An iris plug would normally be inserted to limit the exit aperture to about one centimeter square. The front section of the plug is supported in a steel housing and is pivoted so that it can be rotated about its axis to close the collimator when the diffraction unit is not in use. A reversible motor and gear drive are used to rotate this section. Microswitches are installed between the sections to provide open and closed limit signals. A red beacon is provided to warn personnel in the area when the collimator is not completely closed and that the area is hazardous.

The rear section of the collimator is stationary. A drive shaft and conduit for the switch wires pass through this section in addition to the open passage. The conduit is spiraled to avoid streaming. The drive shaft is straight, but it is positioned so that it is never in line with the opening in the front section.



Vertical Cross Section of Collimator

Figure 6

Section BB

Section CC

Collimator Sections

Figure 7

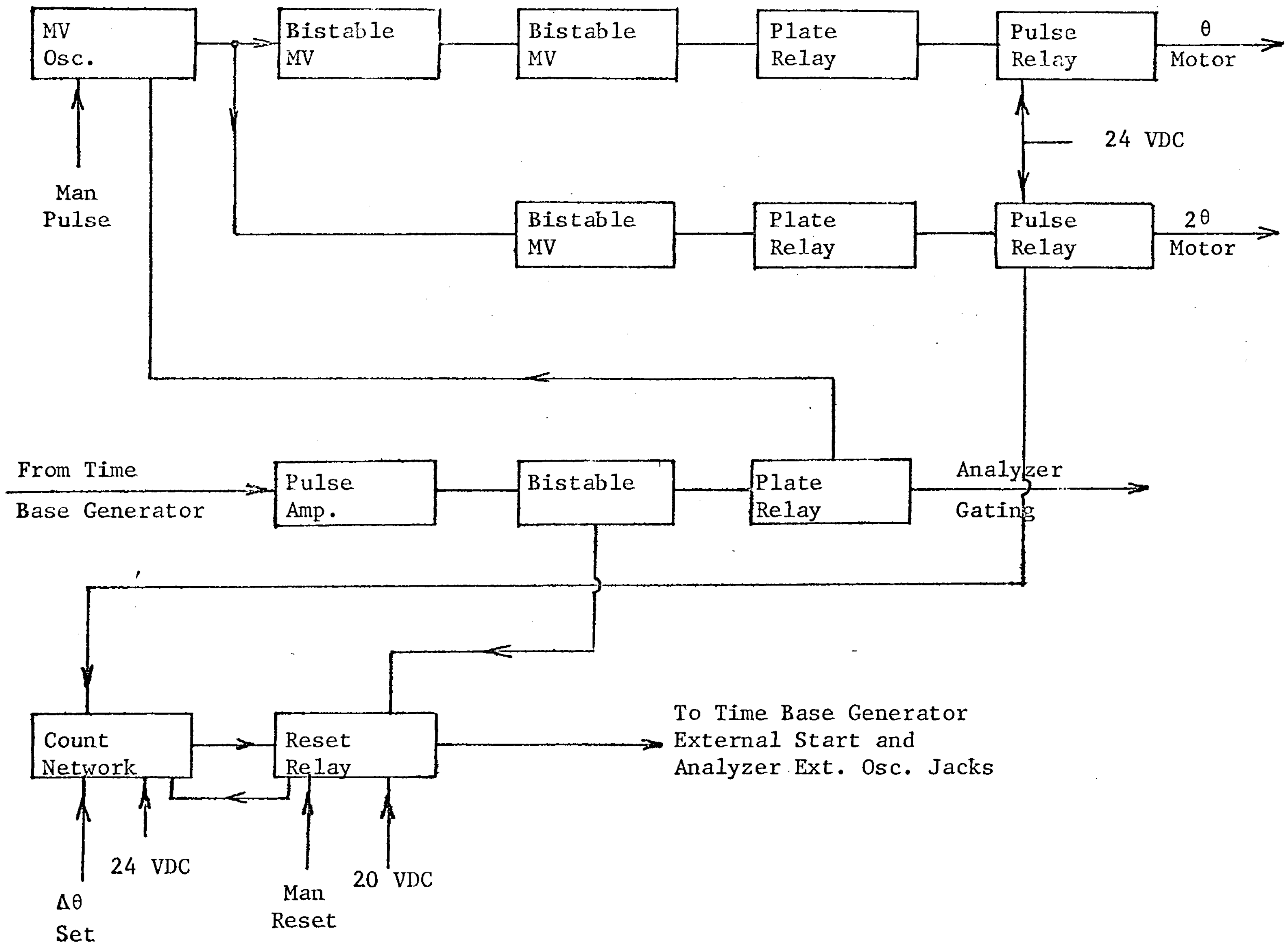
Both sections are filled with magnetite concrete. This provides much better shielding than normal concrete. Eight 3/8-inch-thick lead sheets were placed in front of the collimator to reduce the gamma radiation escaping when the collimator is in use. Some neutron scattering occurs in the lead but this scattering is within tolerable limits.

A borated paraffin beam catcher was provided to attenuate the neutron beam which passes through the crystal. The portion of the beam catcher in the main beam has approximately 0.5 pound of boric acid per pound of paraffin. The side walls have about 0.25 pound of boric acid per pound of paraffin.

No provisions are presently provided for gamma attenuation. The gamma beam is presently dissipated into the concrete wall of the beam room.

A system of controls has been constructed which allows automatic operation of the diffractometer. A block diagram of the control system is shown in Figure 8. An RIDL 400 channel analyzer is used for data storage. The system is designed to take a count for up to 800 seconds, stop data storage in the analyzer, advance the crystal through an angle $\Delta\theta$ and the detector through an angle $2\Delta\theta$, advance the analyzer to a new channel and restart the time base generator.

Due to the method of interconnecting to the analyzer, one channel advance occurs at the end of the predetermined time and another occurs at the start of the next counting interval. Therefore, only alternate channels will contain useful data. A 2:1 ratio is obtained by using DC pulse motors with a 2:1 pulse ratio.



Control Circuit Block Diagram

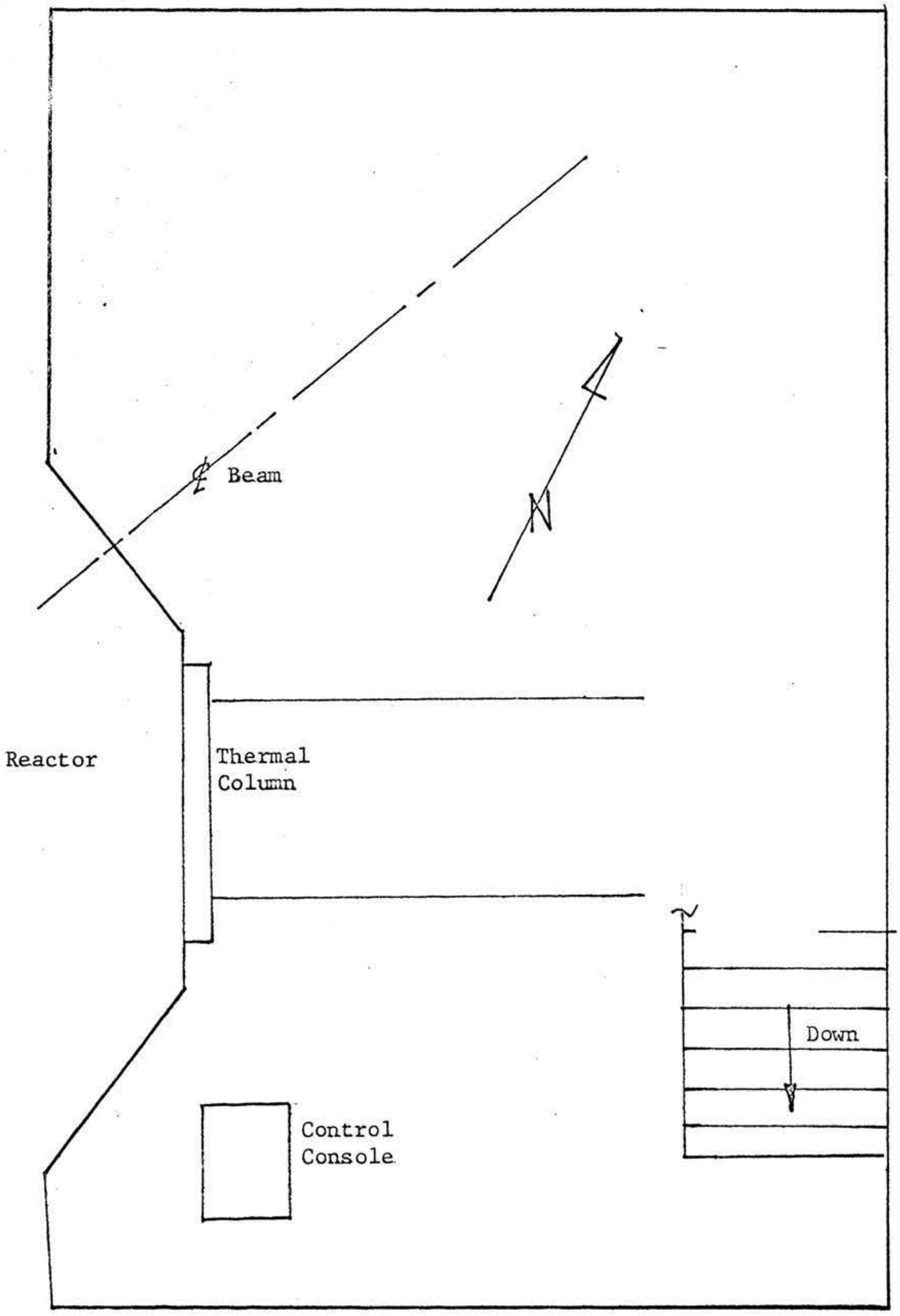
Figure 8

III. DATA AND RESULTS

Preliminary runs were made before the crystal goniometer was installed. The purpose of the first run was to conduct a radiation survey to evaluate the radiation hazards in the area. It was found that at 10 kilowatts the gamma radiation level at the collimator exit was 5 rem per hour. The level behind the neutron beam catcher was less than 20 millirem per hour. The neutron radiation level was approximately 10,000 counts per minute at one kilowatt as measured with Nuclear Chicago Model 2112 Neutron Monitor, which corresponds to a dose rate of 5.1 rem per hour. Assuming a linear relationship which is nearly true, this would correspond to a dose rate of 51 rem per hour at 10 kilowatts. There was no indication of neutrons behind the beam catcher. There was also no indication of neutrons or gamma rays outside the primary beam.

The purpose of the next three runs was to obtain rocking crystal curves. A large copper crystal was used. The crystal was set on edge on a concrete block which was placed on the crystal table. No provisions were made to orient the crystal planes parallel to the vertical. Approximate alignment was made by eye. The detector arm with the one inch RCL BF_3 tube in position was fixed at an angle of about 45 degrees*. The first run indicated only that a peak did occur. During the first run the face of the detector shield was about 30 inches from the crystal. Considerable neutron scattering was observed. The dose rate at some points about 4 feet from the crystal and outside the secondary beam exceeded 100 millirem per hour. No gamma-ray scatter was observed. The total dose in the region where the controls were located (see Figure 9) was at times as high as 10 millirem per hour.

*All angles are measured from the primary neutron beam.



Beam Room Floor Plan

Figure 9

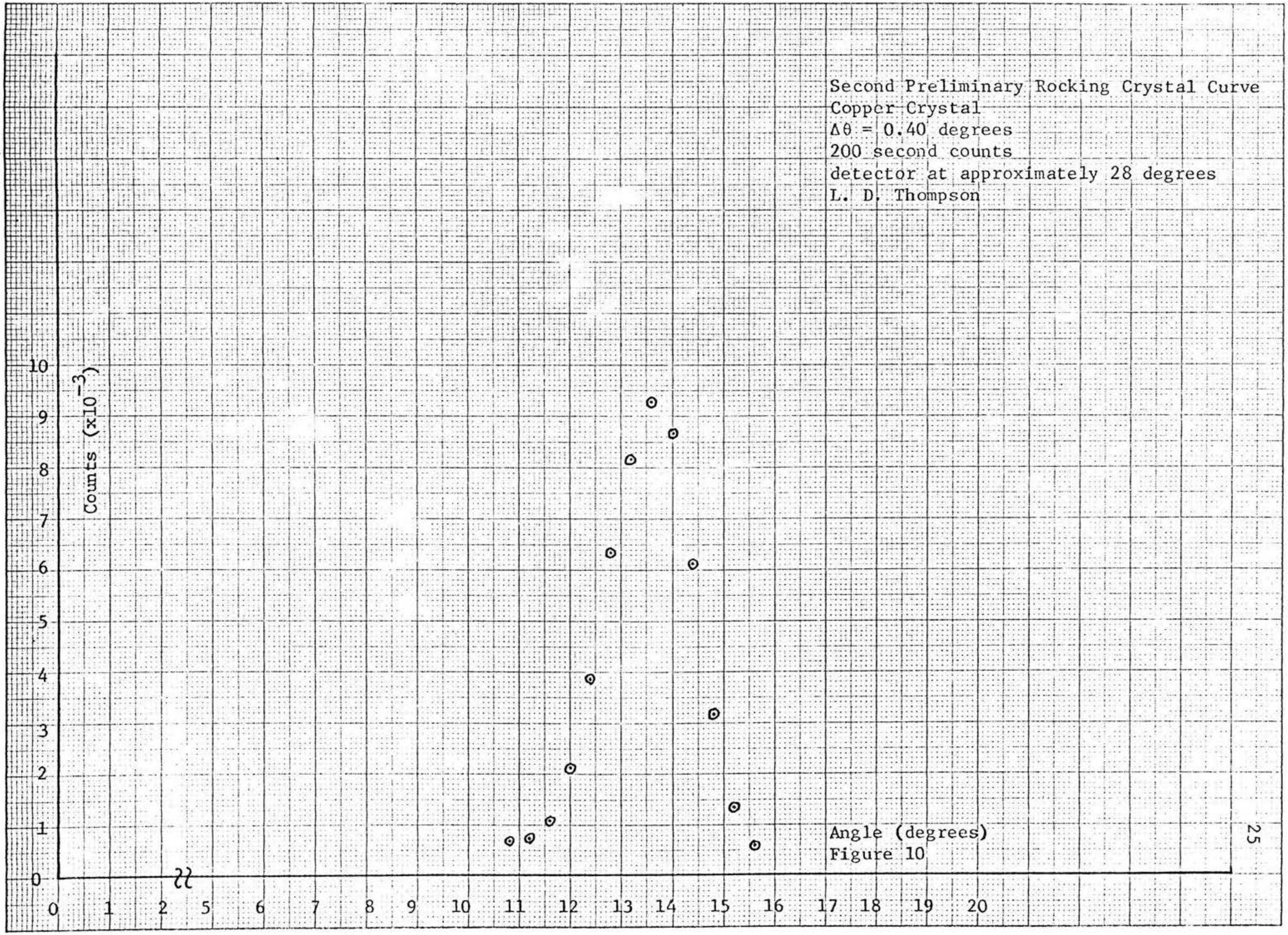
The total dose rate in all other regions of the reactor did not exceed normal background.

The second rocking crystal curve was run with an angle increment of 0.40 degrees. The detector arm was fixed at approximately 50 degrees and the face of the detector shield was about 9 inches from the crystal. The results of the run are shown in Figure 10. The curve is of the shape expected.

A third rocking crystal curve, which was a repeat of the second, was run with an angle increment of 0.10 degrees. The other parameters were held constant. The interconnection between the control unit and the analyzer was changed between the second and third run. This was done to provide data storage in every channel rather than in alternate channels as was the case for the first two runs.

The curve obtained is shown in Figure 11. This curve gives a full width at half maximum of 2.0 degrees.

The crystal was then moved back to the position which corresponded to the peak of the rocking crystal curve. The crystal table and the detector arm were then rotated to a crystal position of 5.0 degrees using the $\theta - 2\theta$ drive. A $\theta - 2\theta$ curve was then started using an increment of 0.50 degrees. The analyzer stopped functioning after 16 points had been taken due to a blown fuse; however, the analyzer functioned properly after the fuse was replaced. As the failure was not discovered immediately, the controls were stopped and the crystal table was backed up 6.00 degrees to get overlap between the two curves. The controls were then restarted. The reactor was shutdown during the thirty-seventh count due to operational difficulties. The curve obtained is shown in Figure 12.


Second Preliminary Rocking Crystal Curve
Copper Crystal
Δθ = 0.40 degrees
200 second counts
detector at approximately 28 degrees
L. D. Thompson
Counts (x10^{-3})
0
1
2
3
4
5
6
7
8
9
10
0
1
2
5
6
7
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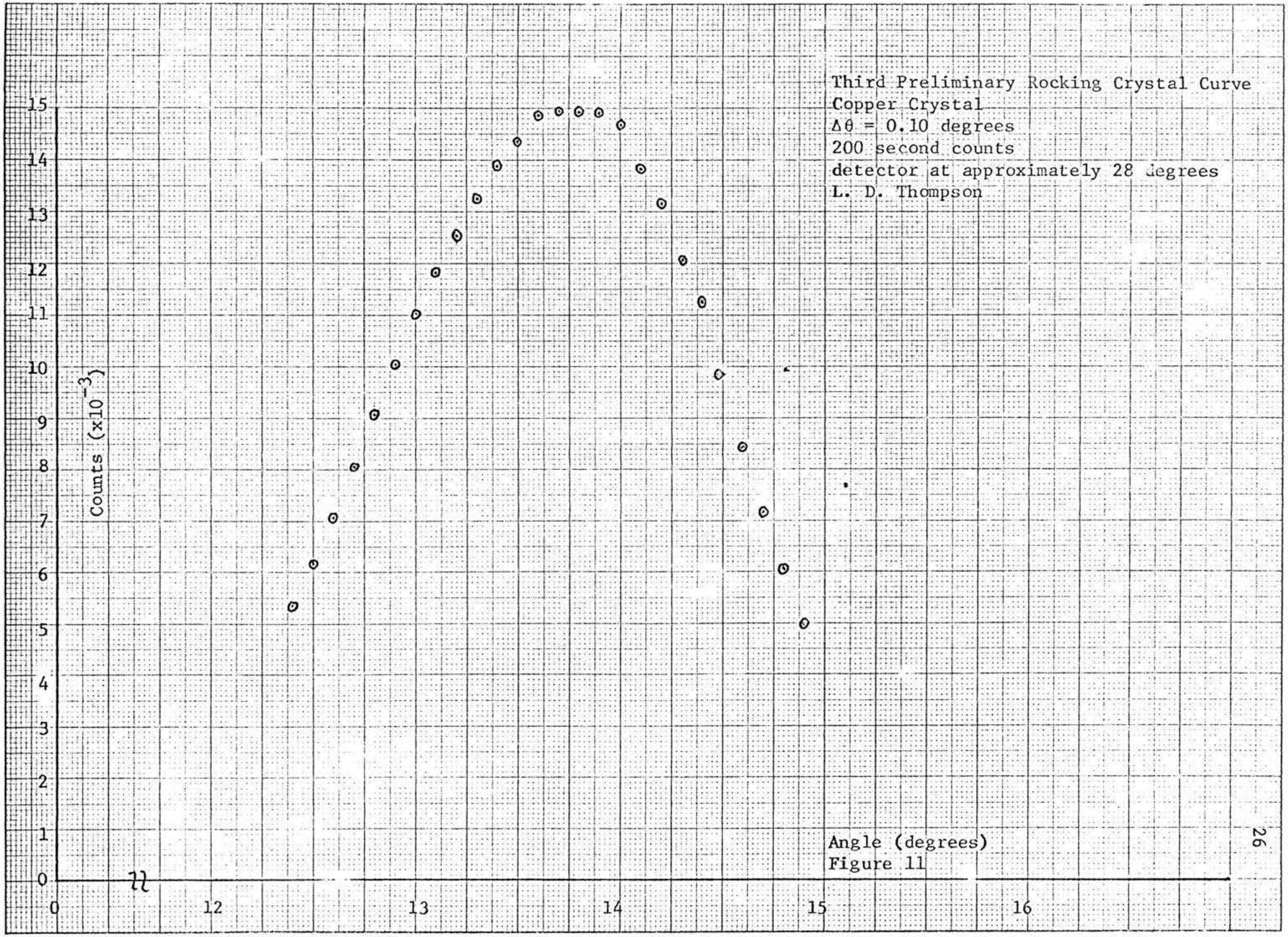
18
19
20
Angle (degrees)
Figure 10


Third Preliminary Rocking Crystal Curve
Copper Crystal
$\Delta\theta$ = 0.10 degrees
200 second counts
detector at approximately 28 degrees
L. D. Thompson
Counts ($\times 10^{-3}$)
0
1
2
3
4
5
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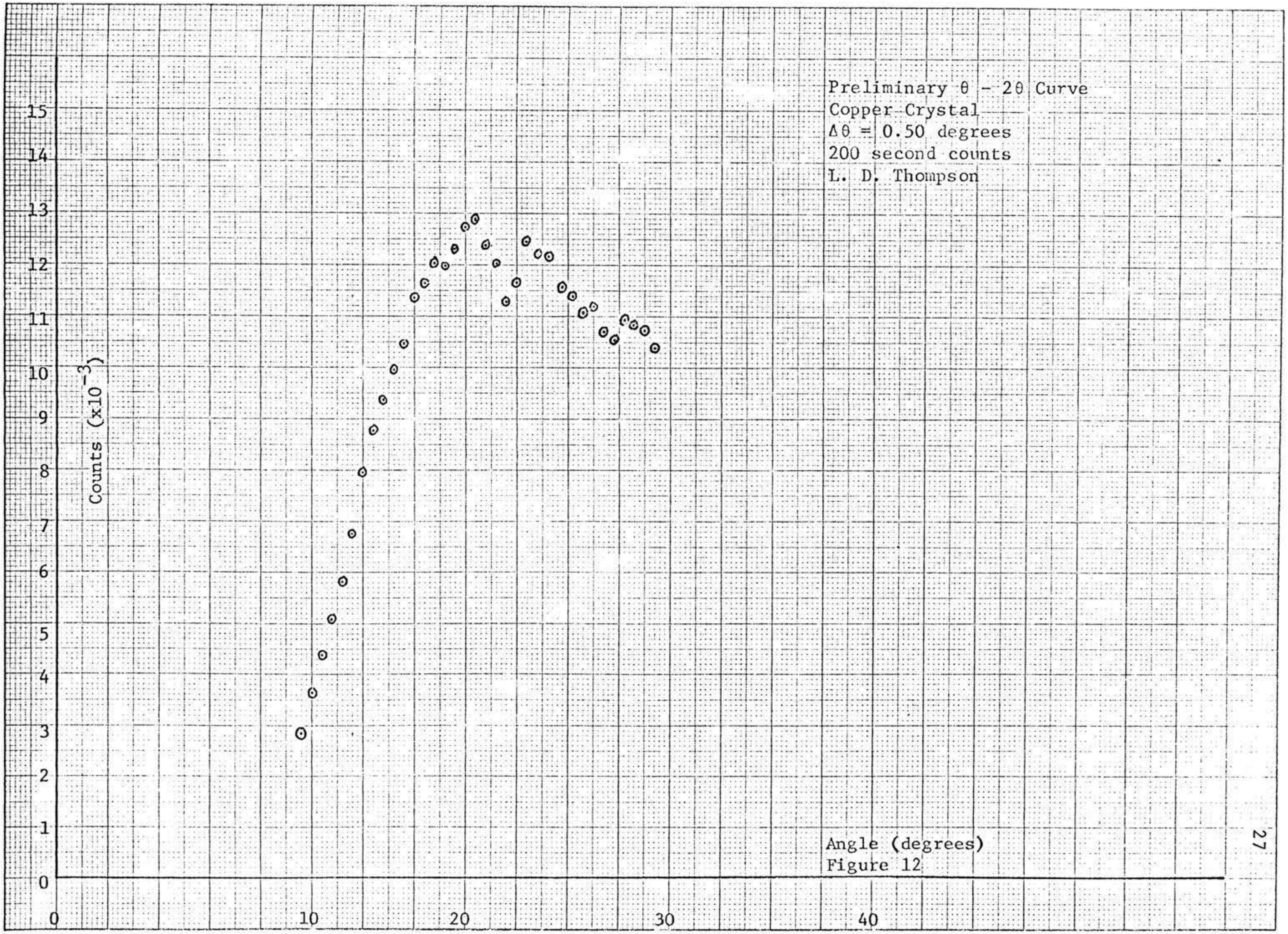
12
13
14
15
16
Angle (degrees)
Figure 11


Preliminary θ - 2θ Curve
Copper Crystal
Δθ = 0.50 degrees
200 second counts
L. D. Thompson
Counts (x10^-3)
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
0
10
20
30
40
Angle (degrees)
Figure 12

The first portion of the curve is about as expected. However, the upper portion of the curve is erratic and does not follow predicted results.

The goniometer was then installed on the crystal table with the lithium flouride crystal in place. The face of the crystal was then centered over the axis of rotation of the crystal table.

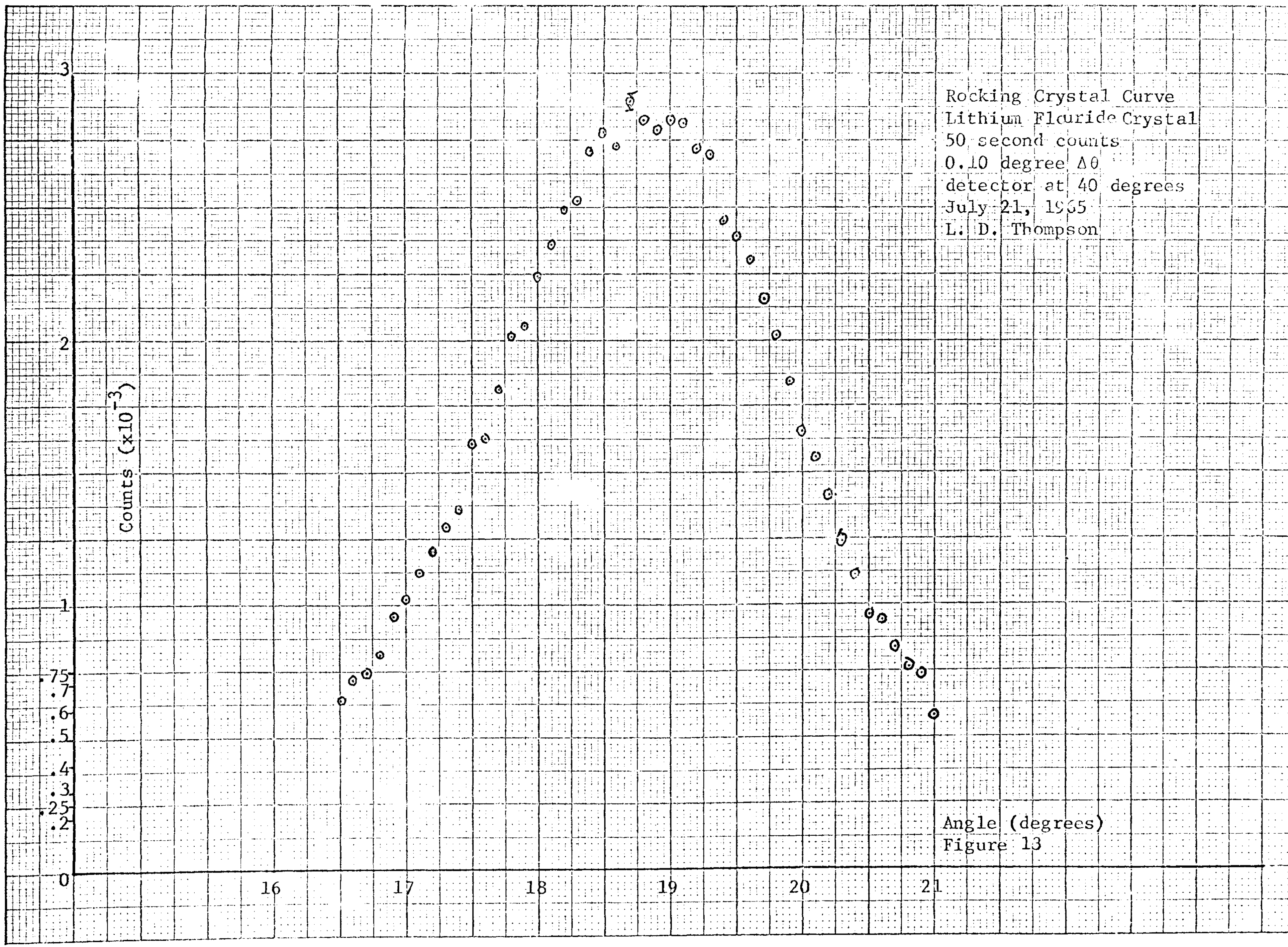
A rocking crystal curve and a θ - 2θ curve were run. Both curves followed the predicted curves closely. The rocking crystal curve is shown in Figure 13 and the θ - 2θ curve is shown in Figure 14*. The rocking crystal curve gives a width at one-half maximum of 2.7 degrees. The curve was run using an angle increment of 0.10 degrees.

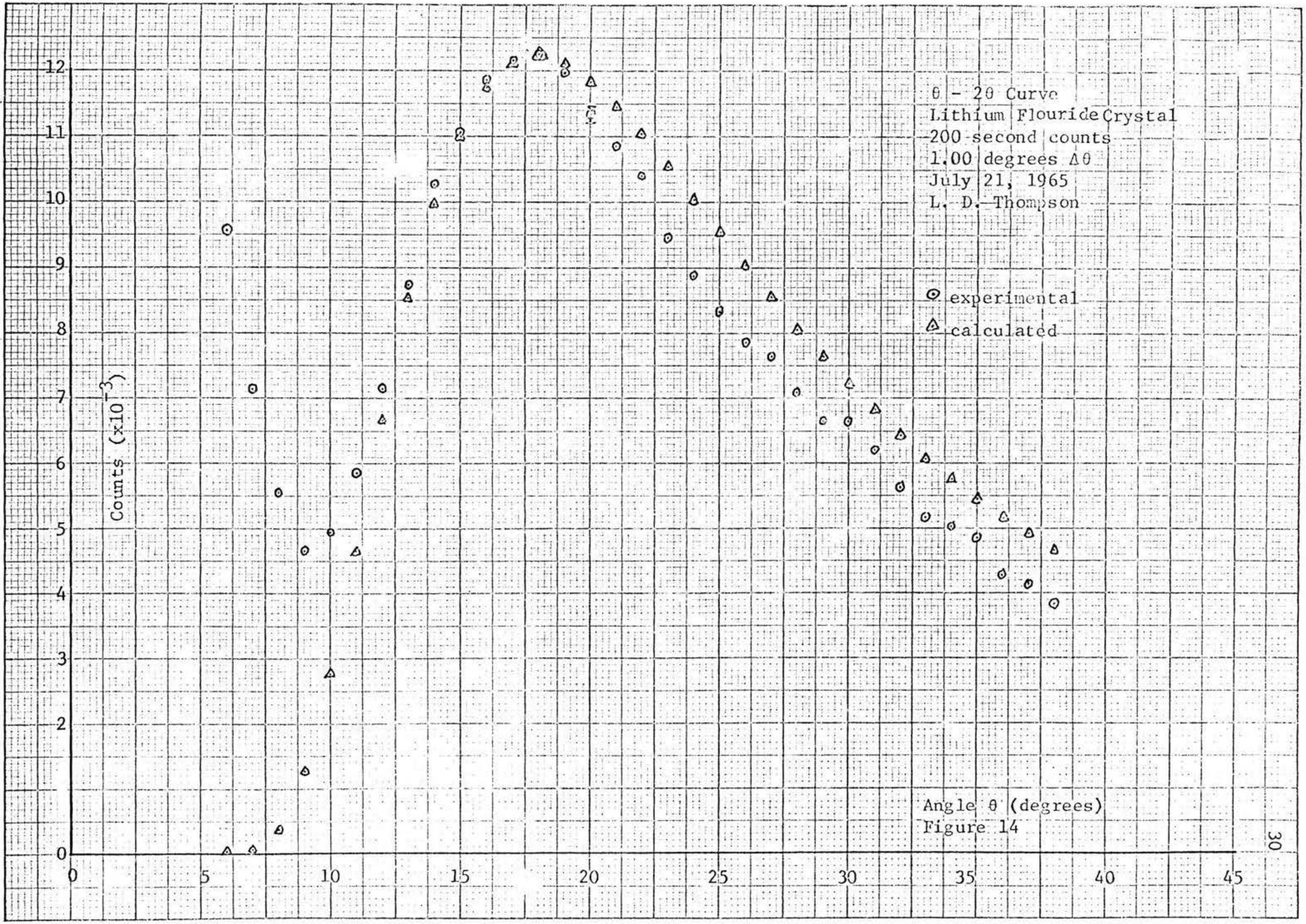
A theoretical Maxwell-Boltzmann curve normalized to the peak of the θ - 2θ curve was calculated. This curve is also shown in Figure 14. A comparison of these two curves shows that the actual spectrum does follow the theoretical spectrum quite closely. The θ - 2θ curve was not correct for background.

A rocking crystal curve using the copper crystal was then run. This curve was much the same as previous curves using a 0.10 angle increment. The width at one-half maximum was approximately 3.2 degrees.

During the repositioning of the crystal table and detector arm, the pulse counting network failed. As a result, synchronization between the position of the crystal table and the detector arm was lost. This made it necessary that the rocking crystal curve be re-run in order to determine the proper position for the crystal table with respect to the detector arm. This would not have been necessary if accurate angle readout were available.

*Data and theoretical calculations are given in Appendix I.


Rocking Crystal Curve
Lithium Flcuride Crystal
50 second counts
0.10 degree Δθ
detector at 40 degrees
July 21, 1965
L. D. Thompson
Counts (x10^-3)
3
2
1
.75
.7
.6
.5
.4
.3
.25
.2
0
16
17
18
19
20
21
Angle (degrees)
Figure 13


θ - 2θ Curve
Lithium Flouride Crystal
200 second counts
1.00 degrees Δθ
July 21, 1965
L. D. Thompson
experimental
calculated
Counts (x10^-3)
0
2
3
4
5
6
7
8
9
10
11
12
0
5
10
15
20
25
30
35
40
45
Angle θ (degrees)
Figure 14

Another rocking crystal curve was obtained. The results of this curve are shown in Figure 15. The width at one-half maximum was again approximately 3.2 degrees. The crystal was then rotated back to the peak of the curve and the crystal table and arm were then repositioned to a crystal angle of 5 degrees for the start of the $\theta - 2\theta$ curve.

The $\theta - 2\theta$ curve is shown in Figure 16. A theoretical Maxwell-Boltzman curve normalized to the peak of the experimental curve is also shown in this figure.

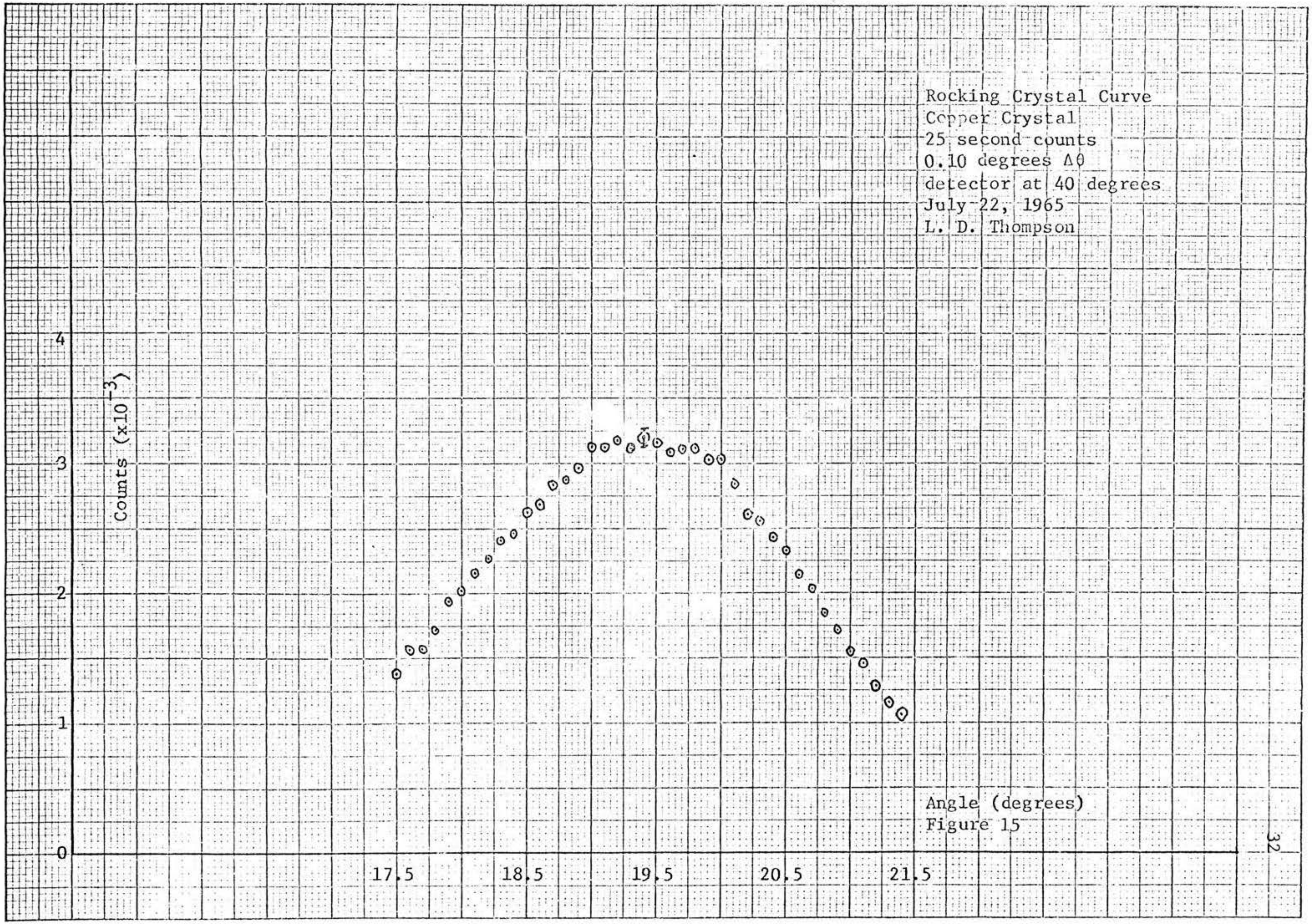
The standard deviation is shown on the curves at five degree intervals. The standard deviation at the other intervals is of the same order.

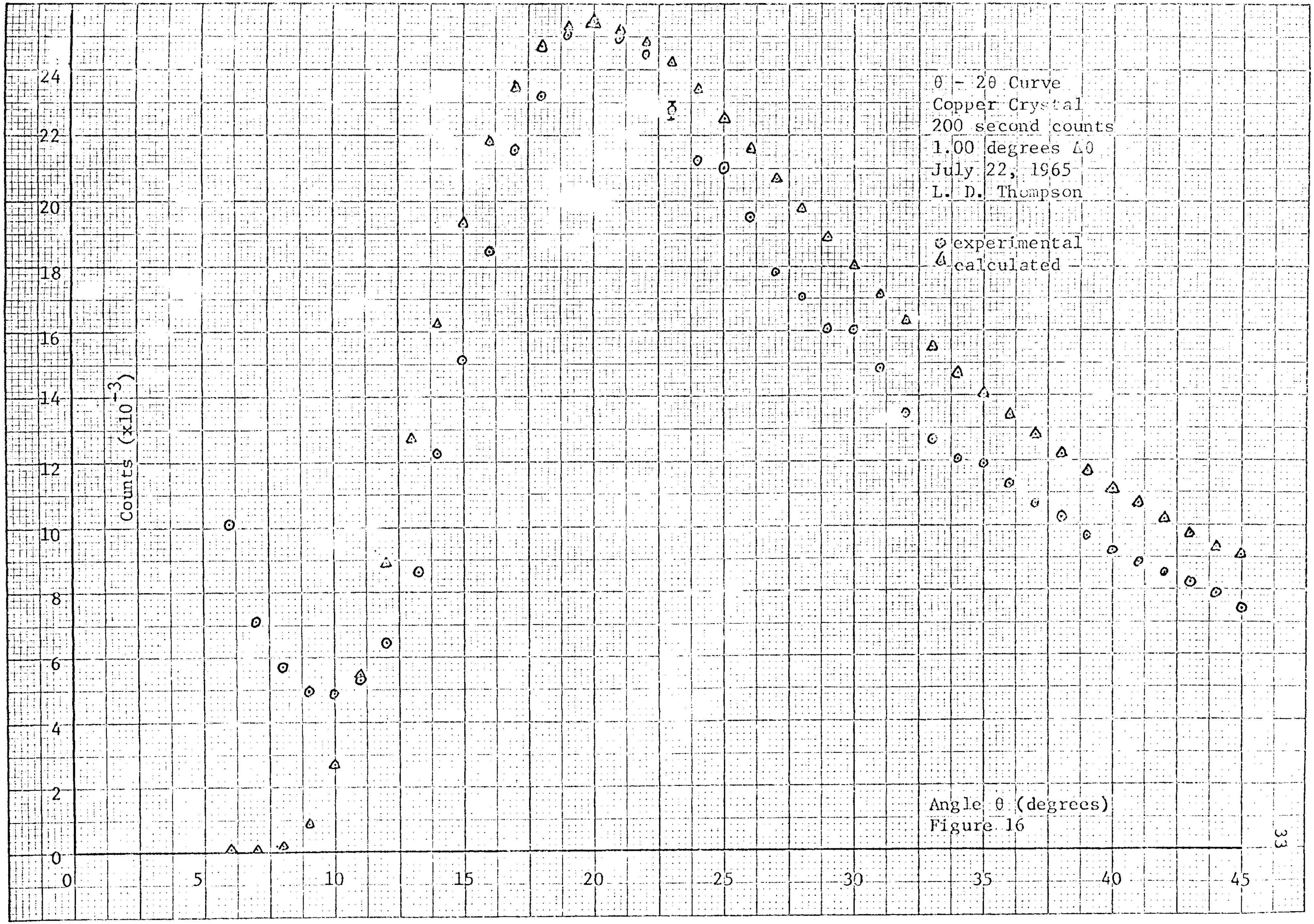
The spectrum curves show that the experimental curves agree well with the calculated curve. The deviation in the lower regions can be explained by increased non-coherent scattering from the crystal at low angles. This effect would be greatly reduced if the curve has been corrected for background. Correction for background using the offset crystal technique described earlier would also result in better agreement in the higher angle regions, although this is best explained by the decrease in the reflectivity of the crystals with increasing neutron energy (angle).

The reflectivity, R, is given by the expression

$$R = \frac{N_c \lambda^2 F}{\sin 2\theta} \tanh (N_c \lambda t_0 F/\sin \theta)$$

where N_c is the number of unit cells per unit volume, is the neutron wavelength, F is the structure factor of a unit cell, t_0 is the crystal thickness and θ is the incident angle[1].


Rocking Crystal Curve
Copper Crystal
25 second counts
0.10 degrees Δθ
detector at 40 degrees
July 22, 1965
L. D. Thompson
Counts (x10^-3)
0
1
2
3
4
17.5
18.5
19.5
20.5
21.5
Angle (degrees)
Figure 15



θ - 2θ Curve
Copper Crystal
200 second counts
1.00 degrees Δθ
July 22, 1965
L. D. Thompson
experimental
calculated
Counts (x10^-3)
Angle θ (degrees)
0
2
4
6
8
10
12
14
16
18
20
22
24
0
5
10
15
20
25
30
35
40
45

Figure 16

The temperature of the neutron beam can be calculated from the equation

$$T_B = \frac{1/2\ m\ (2V_0^{\ 2})}{3/2K}$$

where T_B is the beam temperature (°K), m is the mass of the neutron, V_0 is the most probable velocity, K is a constant described by the equation

$$K = \left. \frac{\frac{C}{\cos\ \theta}}{v^3\ e^{-\left(\frac{v}{v_0}\right)^2}} \right|_V$$

θ is the crystal angle, V is the velocity corresponding to the peak of the θ - 2θ curve.

For the lithium flouride curve, the peak occured at 18° which corresponds to a velocity of 2761 meters per second (see Appendix II). The constant K is found to be 3.42×10^{-7}. The beam temperature (T_B) is then found to be 429 degrees Kelvin or 156 degrees centigrade.

The neutron temperature (T_C) of the moderator at the point of extraction of the neutron beam is given by the expression

$$T_C = \frac{1/2\ m(3/2\ V_0^{\ 2})}{3/2K}$$

where the terms are the same as in the previous equations. From this equation the core neutron temperature (T_C) is calculated to be 347 degrees Kelvin or 74 degrees centigrade. The pool temperature is normally approximately 26 degrees centigrade. This results in a 48 degree centigrade difference between the moderator temperature and the core neutron temperature. As was stated previously this difference normally varies from 50 to 150 degrees centigrade. This indicates that the core neutron temperature obtained is of the order expected.

There are several possible sources of error in these experiments. Among these are crystal table and detector position, variation in counting time due to error in times and detector gating, and variation in neutron flux at the crystal. Of these, the variation in neutron flux is probably the largest single source of error. The total error due to all of these possibilities is estimated to be less than 3%.

IV. CONCLUSIONS

The rocking crystal curves and the spectrum curves are of the shape desired and expected. The lithium flouride rocking crystal curve has a width at one-half maximum of 2.7 degrees. The copper crystal has a width at one-half maximum of 3.2 degrees. These would be reduced if a large distance between crystal and detector was used. This would reduce the effects of using a large detector. These widths could also be reduced by using a Soller collimator.

The unit appears to be performing well with the exception of the pulse counting network and the position indicators. These systems will require close supervision and possible replacement in the near future.

There is very little slack in the drive mechanism. The motors appear adequate to drive the detector arm and crystal table.

In general the unit appears to be very good for the cost involved. The unit provides automatic controls and automatic data storage. The unit is simple enough to operate to make it useful in laboratory classes, but it is still accurate enough to be suitable for graduate research. It appears that the design criterion have been met and the work involved was, in general, a success.

The θ - 2θ curves obtained are in first approximation the neutron spectrum at the beam port. To obtain a more accurate spectrum, corrections should be made for neutron background, changes in crystal reflectivity with neutron energy, and correction for the area of the crystal illuminated by the beam. The neutron background and reflectivity have been previously mentioned. The correction for area of illumination is a simple geometry factor. The area of illumination is more important when small crystals are used than when large crystals are used.

V. RECOMMENDATIONS

The equipment constructed performs well for the money that has been invested. There are modifications which can be made to improve the operation of the unit and its accuracy.

One modification which is necessary for continued automatic operation is the replacement of the pulse counting network which is used to determine the $\Delta\theta$ angle through which the crystal is rotated between counts. Three 11 position stepping relays with associated circuitry are presently used for this purpose. Trouble was encountered with this circuit during the last copper crystal runs. It appeared that the counting circuit failed due to corrosion on the wiper arms of the stepping relay. These relays will require a great deal of service if they are not replaced by a new system. It is recommended that these relays be replaced by the glow tube counter system used by Argonne National Laboratory as described in their drawings #EL-D-3057Q. A second but far less desirable replacement is a preset electro-mechanical counter.

No accurate cost estimate is available for the glow tube counting system. The cost would probably be on the order of $125 to $200.

A new system would provide angle increments as small as 0.01 degrees. The smallest angle increment now available is 0.10 degree. This would greatly improve the accuracy of the system.

A second modification which is needed for accurate and reproducible results is shaft position digitizers. These shaft position digitizers would be used to replace the selsyns now used for remote angle readout. The selsyns now used would at best give an accuracy of ± 0.05 degree. The selsyns are completely unreliable now due to the high drag in the digital indicators used.

Two shaft position digitizers would be needed; one for the crystal table drive and one for the detector arm drive. These digitizers should provide 100 accurate position indications per revolution of the input shaft, and they should have a range of ± 100 revolutions from a zero position. This would provide adequate indication since the minimum possible increment of $\frac{1}{100}$ revolution which corresponds to 0.01 degree rotation of crystal table or detector arm. One hundred revolutions would correspond to 100 degrees which is greater than the maximum travel of the detector arm. No specific digitizer is recommended, rather it is recommended that Mr. Mueller of Argonne National Laboratory be contacted for information as to what digitizers are in use with their units.

A third modification which would increase the range of the unit would be to relocate the crystal table and the detector arm drive mechanism approximately 20 degrees clockwise (looking down on the unit) from its present location. This would not decrease the detector arm travel in the $-\theta$ direction and it would increase the detector arm travel approximately 10 degrees in the $+\theta$ direction.

The drives are not permanently mounted. They could be relocated now with a minimum of additional work and cost.

Another modification that is needed is to replace the wood detector shield mount with a similar mount made of metal. The new mount should be made to fit the detector arm closer than the present mount.

Two other modifications that would improve the accuracy of the unit is the use of a Soller Collimator and a new iris plug with a smaller opening.

APPENDIX I

Table 1

Computer Program for the Calculation of Theoretical Spectrum for LiF Crystal with Output

```
C       CALCULATION OF THEORETICAL SPECTRUM FOR LiF CRYSTAL
        DIMENSION F(200),ANG(200)
        VMP=2760.
        VO=VMP/1.22
        FMP=12226.
        C=FMP*EXPF(1.22**2.)/(VMP**3.)
        DO 10 I=6,136
        A=I
        ANG(I)=A-1.0
        B=ANG(I)*3.14116/180.00
        V=0.851E+03/SINF(B)
   10   F(I)=C*(V**3.)/(EXPF(V**2.)/(VO**2.))
        PRINT 100
        PRINT 200,(ANG(I),F(I),I=6,136)
  100   FORMAT (6X5HANGLE15X1HF)
  200   FORMAT (2E18.8)
        CALL EXIT
        END
```

Table 1 (Cont.)

Angle	F
.50000000E+01	.19490367E-01
.60000000E+01	.33012298E+01
.70000000E+01	.63886791E+02
.80000000E+01	.39569155E+03
.90000000E+01	.12781151E+04
.10000000E+02	.27780829E+04
.11000000E+02	.46887434E+04
.12000000E+02	.66909147E+04
.13000000E+02	.85127298E+04
.14000000E+02	.99934084E+04
.15000000E+02	.11075827E+05
.16000000E+02	.11772941E+05
.17000000E+02	.12134860E+05
.18000000E+02	.12225206E+05
.19000000E+02	.12107284E+05
.20000000E+02	.11837305E+05
.21000000E+02	.11461902E+05
.22000000E+02	.11018022E+05
.23000000E+02	.10534000E+05
.24000000E+02	.10030980E+05
.25000000E+02	.95242905E+04
.26000000E+02	.90247544E+04
.27000000E+02	.85397811E+04
.28000000E+02	.80741866E+04
.29000000E+02	.76309109E+04
.30000000E+02	.72114920E+04
.31000000E+02	.68165120E+04
.32000000E+02	.64458378E+04
.33000000E+02	.60989016E+04
.34000000E+02	.57747932E+04
.35000000E+02	.54724321E+04
.36000000E+02	.51906256E+04
.37000000E+02	.49281442E+04
.38000000E+02	.46837420E+04
.39000000E+02	.44562012E+04
.40000000E+02	.42443543E+04
.41000000E+02	.40470829E+04
.42000000E+02	.38633297E+04
.43000000E+02	.36921123E+04
.44000000E+02	.35325061E+04
.45000000E+02	.33836579E+04
.46000000E+02	.32447676E+04
.47000000E+02	.31151123E+04
.48000000E+02	.29940034E+04
.49000000E+02	.28808274E+04
.50000000E+02	.27750085E+04
.51000000E+02	.26760181E+04
.52000000E+02	.25833727E+04
.53000000E+02	.24966242E+04
.54000000E+02	.24153659E+04
.55000000E+02	.23392218E+04

Table 1 (Cont.)

.56000000E+02	.22678438E+04
.57000000E+02	.22009186E+04
.58000000E+02	.21381504E+04
.59000000E+02	.20792733E+04
.60000000E+02	.20240387E+04
.61000000E+02	.19722196E+04
.62000000E+02	.19236078E+04
.63000000E+02	.18780105E+04
.64000000E+02	.18352527E+04
.65000000E+02	.17951696E+04
.66000000E+02	.17576123E+04
.67000000E+02	.17224408E+04
.68000000E+02	.16895322E+04
.69000000E+02	.16587650E+04
.70000000E+02	.16300350E+04
.71000000E+02	.16032426E+04
.72000000E+02	.15782966E+04
.73000000E+02	.15551151E+04
.74000000E+02	.15336203E+04
.75000000E+02	.15137429E+04
.76000000E+02	.14954205E+04
.77000000E+02	.14785925E+04
.78000000E+02	.14632085E+04
.79000000E+02	.14492196E+04
.80000000E+02	.14365827E+04
.81000000E+02	.14252610E+04
.82000000E+02	.14152197E+04
.83000000E+02	.14064283E+04
.84000000E+02	.13988598E+04
.85000000E+02	.13924942E+04
.86000000E+02	.13873101E+04
.87000000E+02	.13832930E+04
.88000000E+02	.13804327E+04
.89000000E+02	.13787198E+04
.90000000E+02	.13781506E+04
.91000000E+02	.13787211E+04
.92000000E+02	.13804340E+04
.93000000E+02	.13832957E+04
.94000000E+02	.13873112E+04
.95000000E+02	.13924966E+04
.96000000E+02	.13988636E+04
.97000000E+02	.14064307E+04
.98000000E+02	.14152234E+04
.99000000E+02	.14252664E+04
.10000000E+03	.14365879E+04
.10100000E+03	.14492248E+04
.10200000E+03	.14632152E+04
.10300000E+03	.14785992E+04
.10400000E+03	.14954270E+04
.10500000E+03	.15137513E+04
.10600000E+03	.15336286E+04
.10700000E+03	.15551247E+04
.10800000E+03	.15783064E+04

Table 1 (Cont.)

.10900000E+03	.16032526E+04
.11000000E+03	.16300467E+04
.11100000E+03	.16587784E+04
.11200000E+03	.16895440E+04
.11300000E+03	.17224562E+04
.11400000E+03	.17576263E+04
.11500000E+03	.17951852E+04
.11600000E+03	.18352707E+04
.11700000E+03	.18780303E+04
.11800000E+03	.19236280E+04
.11900000E+03	.19722403E+04
.12000000E+03	.20240701E+04
.12100000E+03	.20792965E+04
.12200000E+03	.21381765E+04
.12300000E+03	.22009449E+04
.12400000E+03	.22678730E+04
.12500000E+03	.23392519E+04
.12600000E+03	.24153987E+04
.12700000E+03	.24977580E+04
.12800000E+03	.25834073E+04
.12900000E+03	.26760586E+04
.13000000E+03	.27750505E+04
.13100000E+03	.28808735E+04
.13200000E+03	.29940532E+04
.13300000E+03	.31151633E+04
.13400000E+03	.32448268E+04
.13500000E+03	.33837180E+04

Table 2

Computer Program for the Calculation of

Theoretical Spectrum for Cu Crystal with Output

```
C      CALCULATION OF THEORETICAL SPECTRUM FOR Cu CRYSTAL
       DIMENSION F(200),ANG(200)
       VMP=1786
       VO=VMP/1.22
       FMP=25479.
       C=FMP*EXPF(1.22**2.)/(VMP**3.)
       DO 10 I=6,136
       A=I
       ANG(I)=A-1.0
       B=ANG(I)*3.1416/18.000
       D=(0.395E+04*SQRTF(3.))/11.2
       V=D/SING(B)
    10 V(I)=C*(V**3.)/EXPF(V**2.)/(V)**2.))
       PRINT 100
       PRINT 200,(ANG(I),F(I),I=6,136)
   100 FORMAT (6X5HANGLE15X1HF)
   200 FORMAT (2E18.8)
       CALL EXIT
       END
```

Table 2 (Cont.)

Angle	F
.50000000E+01	.75718479E-03
.60000000E+01	.47463925E+00
.70000000E+01	.20219122E+02
.80000000E+01	.20898165E+03
.90000000E+01	.95894394E+03
.10000000E+02	.26793727E+04
.11000000E+02	.54454790E+04
.12000000E+02	.89502566E+04
.13000000E+02	.12710936E+05
.14000000E+02	.16282280E+05
.15000000E+02	.19361774E+05
.16000000E+02	.21800675E+05
.17000000E+02	.23569466E+05
.18000000E+02	.24713883E+05
.19000000E+02	.25318023E+05
.20000000E+02	.25478968E+05
.21000000E+02	.25291848E+05
.22000000E+02	.24841733E+05
.23000000E+02	.24200825E+05
.24000000E+02	.23428157E+05
.25000000E+02	.22570501E+05
.26000000E+02	.21664117E+05
.27000000E+02	.20736560E+05
.28000000E+02	.19808255E+05
.29000000E+02	.18894079E+05
.30000000E+02	.18004474E+05
.31000000E+02	.17146576E+05
.32000000E+02	.16324959E+05
.33000000E+02	.15542232E+05
.34000000E+02	.14799648E+05
.35000000E+02	.14097386E+05
.36000000E+02	.13434907E+05
.37000000E+02	.12811120E+05
.38000000E+02	.12224636E+05
.39000000E+02	.11673807E+05
.40000000E+02	.11156860E+05
.41000000E+02	.10671988E+05
.42000000E+02	.10217348E+05
.43000000E+02	.97911513E+04
.44000000E+02	.93916536E+04
.45000000E+02	.90171543E+04
.46000000E+02	.86660748E+04
.47000000E+02	.83368859E+04
.48000000E+02	.80281714E+04
.49000000E+02	.77385851E+04
.50000000E+02	.74668711E+04
.51000000E+02	.72118714E+04
.52000000E+02	.69724958E+04
.53000000E+02	.67477236E+04
.54000000E+02	.65366212E+04
.55000000E+02	.63383172E+04

Table 2 (Cont.)

.56000000E+02	.61520027E+04
.57000000E+02	.59769268E+04
.58000000E+02	.58123906E+04
.59000000E+02	.56577647E+04
.60000000E+02	.55124484E+04
.61000000E+02	.53758886E+04
.62000000E+02	.52475809E+04
.63000000E+02	.51270583E+04
.64000000E+02	.50138748E+04
.65000000E+02	.49076390E+04
.66000000E+02	.48079767E+04
.67000000E+02	.47145434E+04
.68000000E+02	.46270189E+04
.69000000E+02	.45451150E+04
.70000000E+02	.44685593E+04
.71000000E+02	.43971060E+04
.72000000E+02	.43305257E+04
.73000000E+02	.42686009E+04
.74000000E+02	.42111451E+04
.75000000E+02	.41579777E+04
.76000000E+02	.41089397E+04
.77000000E+02	.40638765E+04
.78000000E+02	.40226590E+04
.79000000E+02	.39851621E+04
.80000000E+02	.39512790E+04
.81000000E+02	.39209064E+04
.82000000E+02	.38939560E+04
.83000000E+02	.38703565E+04
.84000000E+02	.38500383E+04
.85000000E+02	.38329395E+04
.86000000E+02	.38190139E+04
.87000000E+02	.38082257E+04
.88000000E+02	.38005405E+04
.89000000E+02	.37959381E+04
.90000000E+02	.37944045E+04
.91000000E+02	.37959375E+04
.92000000E+02	.38005399E+04
.93000000E+02	.38082289E+04
.94000000E+02	.38190170E+04
.95000000E+02	.38329455E+04
.96000000E+02	.38500455E+04
.97000000E+02	.38703672E+04
.98000000E+02	.38939663E+04
.99000000E+02	.39209168E+04
.10000000E+02	.39512929E+04
.10100000E+02	.39851760E+04
.10200000E+02	.40226772E+04
.10300000E+02	.40638950E+04
.10400000E+02	.41089571E+04
.10500000E+02	.41579994E+04
.10600000E+02	.42111709E+04
.10700000E+02	.42686270E+04
.10800000E+02	.43305528E+04

Table 2 (Cont.)

.10900000E+03	.43971371E+04
.11000000E+03	.44685909E+04
.11100000E+03	.45451496E+04
.11200000E+03	.46270557E+04
.11300000E+03	.47145800E+04
.11400000E+03	.48080190E+04
.11500000E+03	.49076809E+04
.11600000E+03	.50139227E+04
.11700000E+03	.51271055E+04
.11800000E+03	.52476346E+04
.11900000E+03	.53759433E+04
.12000000E+03	.55125083E+04
.12100000E+03	.56578261E+04
.12200000E+03	.58124591E+04
.12300000E+03	.59769974E+04
.12400000E+03	.61520736E+04
.12500000E+03	.63383962E+04
.12600000E+03	.65367068E+04
.12700000E+03	.67478116E+04
.12800000E+03	.69725932E+04
.12900000E+03	.72119757E+04
.13000000E+03	.74669862E+04
.13100000E+03	.77387016E+04
.13200000E+03	.80282911E+04
.13300000E+03	.83370172E+04
.13400000E+03	.86662161E+04
.13500000E+03	.90173056E+04

Table 3

Data for Rocking Crystal Curve

Lithium Flcuride Crystal

Angle (degrees)	Counts
16.5	636
16.6	718
16.7	743
16.8	814
16.9	951
17.0	1019
17.1	1124
17.2	1200
17.3	1289
17.4	1363
17.5	1603
17.6	1623
17.7	1819
17.8	2014
17.9	2068
18.0	2249
18.1	2357
18.2	2499
18.3	2518
18.4	2705
18.5	2777
18.6	2724
18.7	2892
18.8	2828
18.9	2785
19.0	2823
19.1	2811
19.2	2711
19.3	2698

Table 3 (Cont.)

Data for Rocking Crystal Curve

Lithium Flouride Crystal

Angle (degrees)	Counts
19.4	2444
19.6	2301
19.7	2161
19.8	2023
19.9	1846
20.0	1654
21.1	1567
21.2	1417
21.3	1236
21.4	1112
21.5	964
21.6	945
21.7	832
21.8	765
21.9	748
22.0	576

Table 4

Data for Rocking Crystal Curve

Copper Crystal

Angle (degrees)	Counts
17.5	1388
17.6	1553
17.7	1555
17.8	1717
17.9	1952
18.0	2029
18.1	2159
18.2	2258
18.3	2405
18.4	2453
18.5	2675
18.6	2690
18.7	2845
18.8	2868
18.9	2962
19.0	3130
19.1	3121
19.2	3181
19.3	3129
19.4	3200
19.5	3164
19.6	3090
19.7	3115
19.8	3136
19.9	3025

Table 4 (Cont.)

Data for Rocking Crystal Curve

Copper Crystal

Angle (degrees)	Counts
20.0	3040
20.1	2848
20.2	2666
20.3	2607
20.4	2439
20.5	2337
20.6	2143
20.7	2033
20.8	1839
20.9	1706
21.0	1545
21.2	1497
21.3	1281
21.4	1164
21.5	1057

Table 5

Data for θ - 2θ Curve

Lithium FlourideCrystal

Angle (degrees)	Calculated (counts)	Experimental (counts)
6.00	3.30	9,569
7.00	63.9	7,124
8.00	395	5,541
9.00	1,278	4,671
10.00	2,778	4,963
11.00	4,689	5,851
12.00	6,691	7,147
13.00	8,513	8,746
13.00	9,993	10,279
15.00	11,076	11,415
16.00	11,773	11,887
17.00	12,135	12,178
18.00	12,225	12,226
19.00	12,107	11,994
20.00	11,837	11,335
21.00	11,462	10,853
22.00	11,018	10,402
23.00	10,534	9,467
24.00	10,031	8,895
25.00	9,524	8,314
26.00	9,025	7,872
27.00	8,540	7,650
28.00	8,074	7,082
29.00	7,630	6,670

Table 5 (Cont.)

Data for θ - 2θ Curve

Lithium Flouride Crystal

Angle (degrees)	Calculated (counts)	Experimental (counts)
30.00	7,211	6,679
31.00	6,817	6,202
32.00	6,446	5,625
33.00	6,099	5,187
34.00	5,775	5,005
35.00	5,472	4,857
36.00	5,191	4,273
37.00	4,928	4,109
38.00	4,683	3,809
39.00	4,456	3,923
40.00	4,244	3,801

Table 6

Data for θ - 2θ Curve

Copper Crystal

Angle (degrees)	Calculated (counts)	Experimental (counts)
6.00	0.475	10,100
7.00	20.22	7,108
8.00	209.0	5,720
9.00	958.9	4,991
10.00	2,679	4,862
11.00	5,445	5,281
12.00	8,950	6,451
13.00	12,711	8,604
14.00	16,282	12,328
15.00	19,362	15,173
16.00	21,801	18,443
17.00	23,569	21,587
18.00	24,714	23,185
19.00	25,318	25,023
20.00	25,479	25,479
21.00	24,292	24,963
22.00	24,842	24,473
23.00	24,201	22,759
24.00	23,428	21,229
25.00	22,571	21,058
26.00	21,664	19,504
27.00	20,737	17,866
28.00	19,808	17,207
29.00	18,894	16,066

Table 6 (Cont.)

Data for θ - 2θ Curve

Copper Crystal

Angle (degrees)	Calculated (counts)	Experimental (counts)
30.00	18,004	16,080
31.00	17,147	14,874
32.00	16,325	13,463
33.00	15,542	12,608
34.00	14,800	12,029
35.00	14,974	11,904
36.00	13,435	11,362
37.00	12,811	10,671
38.00	12,225	10,268
39.00	11,674	9,669
40.00	11,157	9,232
41.00	10,672	8,859
42.00	10,217	8,549
43.00	9,791	8,239
44.00	9,392	7,948
45.00	9,017	7,427

APPENDIX II

Table 7

Computer Program for the Calculation of

Wave Length and Velocity as a Function of Angle with Output

```
C       CALCULATION OF WAVE LENGTH AND VELOCITY AS A FUNCTION OF ANGLE
        DIMENSION ANG(200), WLIF(200),WCU(200),VLIF(200),VCU(200)
        ALIF=4.01
        ACU=5.6
        DLIF=ALIF/SWRTF(3.0)
        DCU=ACU/SQRTF(3.0)
        DO 10 I=6,136
        A=I
        ANG(I)=A-1.0
        B=ANG(I)*3.1416/18.000
        WLIF(I)=2.*DLIF*SINF(B)
        WCU(I)=2.*DCU*SINF(B)
        VLIF(I)=0.395E-04/WLIF(I)*0.1E+09
     10 VCU(I)=0.395E-04/WCU(I)*0.1E+09
        PRINT 100
        PRINT 110
        PRINT 120
        PRINT 200,(ANG(I),WLIF(I),VLIF(I),WCU(I),I=6,136)
    100 FORMAT(16X15HLITHIUM FLORIDE14X6HCOPPER)
    110 FORMAT(3XANGLE5X10WAVELENGTH3X8HVELOCITY3X10HWAVELENGTH3X8HVELO
       2CITY)
    120 FORMAT(1X9H(DEGREES)4X23H(ANGSTROMS)METERS/SEC)1X23H(ANGSTROMS)(M
       2ETERS/SEC))
    200 FORMAT(5E12.6)
        CALL EXIT
        END
```

Table 7 (Cont.)

	LITHIUM FLORIDE		COPPER	
ANGLE (DEGREES)	WAVELENGTH (ANGSTROMS)	VELOCITY (METERS/SEC)	WAVELENGTH (ANGSTROMS)	VELOCITY (METERS/SEC)
.500000E+01	.403562E+00	.978782E+04	.563578E+00	.700878E+04
.600000E+01	.484004E+00	.816108E+04	.675916E+00	.584391E+04
.700000E+01	.564298E+00	.699983E+04	.788048E+00	.501238E+04
.800000E+01	.644421E+00	.612952E+04	.899940E+00	.438918E+04
.900000E+01	.724347E+00	.545318E+04	.101155E+01	.390486E+04
.100000E+02	.804053E+00	.491260E+04	.112286E+01	.351777E+04
.110000E+02	.883514E+00	.447078E+04	.123383E+01	.320129E+04
.120000E+02	.962705E+00	.410301E+04	.134442E+01	.293805E+04
.130000E+02	.104160E+01	.379222E+04	.145460E+01	.271550E+04
.140000E+02	.112018E+01	.352620E+04	.156434E+01	.252501E+04
.150000E+02	.119842E+01	.329599E+04	.167361E+01	.236016E+04
.160000E+02	.127629E+01	.309488E+04	.178236E+01	.221615E+04
.170000E+02	.135378E+01	.291774E+04	.189057E+01	.208931E+04
.180000E+02	.143085E+01	.276057E+04	.199820E+01	.197677E+04
.190000E+02	.150749E+01	.262023E+04	.210523E+01	.187627E+04
.200000E+02	.158367E+01	.249419E+04	.221161E+01	.178602E+04
.210000E+02	.165937E+01	.238041E+04	.231732E+01	.170454E+04
.220000E+02	.173456E+01	.227723E+04	.242233E+01	.163065E+04
.230000E+02	.180922E+01	.218325E+04	.252659E+01	.156336E+04
.240000E+02	.188333E+01	.209734E+04	.263009E+01	.150184E+04
.250000E+02	.195687E+01	.201852E+04	.273279E+01	.144540E+04
.260000E+02	.202981E+01	.194598E+04	.283465E+01	.139346E+04
.270000E+02	.210213E+01	.187903E+04	.293565E+01	.134552E+04
.280000E+02	.217382E+01	.181707E+04	.303576E+01	.130115E+04
.290000E+02	.224484E+01	.175958E+04	.313494E+01	.125999E+04
.300000E+02	.231517E+01	.170613E+04	.323316E+01	.122171E+04
.310000E+02	.238481E+01	.165631E+04	.333040E+01	.118604E+04
.320000E+02	.245371E+01	.160980E+04	.342663E+01	.115273E+04
.330000E+02	.252187E+01	.156629E+04	.352181E+01	.112157E+04
.340000E+02	.258926E+01	.152553E+04	.361592E+01	.109238E+04
.350000E+02	.265586E+01	.148727E+04	.370893E+01	.106499E+04
.360000E+02	.272165E+01	.145132E+04	.380081E+01	.103925E+04
.370000E+02	.278771E+01	.141748E+04	.389153E+01	.101502E+04
.380000E+02	.285073E+01	.138560E+04	.398107E+01	.992194E+03
.390000E+02	.291397E+01	.135553E+04	.406939E+01	.970659E+03
.400000E+02	.297633E+01	.132713E+04	.415648E+01	.950323E+03
.410000E+02	.303778E+01	.130028E+04	.424229E+01	.931099E+03
.420000E+02	.309831E+01	.127488E+04	.432682E+01	.912910E+03
.430000E+02	.315789E+01	.125083E+04	.441002E+01	.895685E+03
.440000E+02	.321651E+01	.122803E+04	.449189E+01	.879361E+03
.450000E+02	.327415E+01	.120641E+04	.457238E+01	.863880E+03
.460000E+02	.333080E+01	.118590E+04	.465149E+01	.849189E+03
.470000E+02	.338642E+01	.116642E+04	.472917E+01	.835240E+03
.480000E+02	.344102E+01	.114791E+04	.480542E+01	.821988E+03
.490000E+02	.349457E+01	.113032E+04	.488020E+01	.809392E+03
.500000E+02	.354705E+01	.111359E+04	.495349E+01	.797416E+03
.510000E+02	.359846E+01	.109769E+04	.502528E+01	.786025E+03
.520000E+02	.364877E+01	.108255E+04	.509554E+01	.775187E+03

Table 7 (Cont.)

.530000E+02	.369796E+01	.106815E+04	.516424E+01	.764874E+03
.540000E+02	.374603E+01	.105444E+04	.523137E+01	.755059E+03
.550000E+02	.379296E+01	.104140E+04	.529690E+01	.745717E+03
.560000E+02	.383873E+01	.102898E+04	.526083E+01	.736825E+03
.570000E+02	.388334E+01	.101716E+04	.542312E+01	.728362E+03
.580000E+02	.392676E+01	.100591E+04	.548376E+01	.720308E+03
.590000E+02	.396898E+01	.995215E+03	.554272E+01	.712645E+03
.600000E+02	.401000E+01	.985036E+03	.560000E+01	.705356E+03
.610000E+02	.404979E+01	.975356E+03	.565558E+01	.698425E+03
.620000E+02	.408836E+01	.966157E+03	.570943E+01	.691837E+03
.630000E+02	.412567E+01	.957418E+03	.576154E+01	.685580E+03
.640000E+02	.416173E+01	.949123E+03	.581189E+01	.679640E+03
.650000E+02	.419652E+01	.941254E+03	.586048E+01	.674005E+03
.660000E+02	.423003E+01	.933797E+03	.590728E+01	.668665E+03
.670000E+02	.426226E+01	.926737E+03	.595228E+01	.663610E+03
.680000E+02	.429318E+01	.920061E+03	.599547E+01	.658830E+03
.690000E+02	.432280E+01	.913757E+03	.603683E+01	.654315E+03
.700000E+02	.435110E+01	.907814E+03	.607636E+01	.650059E+03
.710000E+02	.437808E+01	.902220E+03	.611403E+01	.646054E+03
.720000E+02	.440372E+01	.896967E+03	.614984E+01	.642292E+03
.730000E+02	.442802E+01	.892044E+03	.618378E+01	.638767E+03
.740000E+02	.445098E+01	.887444E+03	.621583E+01	.635473E+03
.750000E+02	.447257E+01	.883159E+03	.624599E+01	.632405E+03
.760000E+02	.449281E+01	.879182E+03	.627425E+01	.629557E+03
.770000E+02	.451167E+01	.875506E+03	.630059E+01	.626924E+03
.780000E+02	.452916E+01	.872124E+03	.632502E+01	.624503E+03
.790000E+02	.454527E+01	.869033E+03	.634752E+01	.622290E+03
.800000E+02	.456000E+01	.866226E+03	.636808E+01	.620280E+03
.810000E+02	.457334E+01	.863700E+03	.638671E+01	.618471E+03
.820000E+02	.458528E+01	.861450E+03	.670339E+01	.616860E+03
.830000E+02	.459583E+01	.859473E+03	.641812E+01	.615444E+03
.840000E+02	.460498E+01	.857766E+03	.643090E+01	.614221E+03
.850000E+02	.461273E+01	.856325E+03	.644171E+01	.613190E+03
.860000E+02	.461907E+01	.855150E+03	.645057E+01	.612348E+03
.870000E+02	.462400E+01	.854238E+03	.645746E+01	.611695E+03
.880000E+02	.462752E+01	.853587E+03	.646238E+01	.611229E+03
890000E+02	.462964E+01	.853197E+03	.646533E+01	.610950E+03
.900000E+02	.463034E+01	.853067E+03	.646632E+01	.610857E+03
.910000E+02	.462964E+01	.853197E+03	.646533E+01	.610950E+03
.920000E+02	.462752E+01	.853587E+03	.646238E+01	.611229E+03
.930000E+02	.462400E+01	.854238E+03	.645745E+01	.611695E+03
.940000E+02	.461906E+01	.855150E+03	.645056E+01	.612349E+03
.950000E+02	.461272E+01	.856326E+03	.644171E+01	.613190E+03
.960000E+02	.460498E+01	.857766E+03	.643089E+01	.614222E+03
.970000E+02	.459583E+01	.859474E+03	.641812E+01	.615444E+03
.980000E+02	.458528E+01	.861451E+03	.640338E+01	.616860E+03
.990000E+03	.457333E+01	.863701E+03	.638670E+01	.618472E+03
.100000E+03	.456000E+01	.866228E+03	.636808E+01	.620281E+03
.101000E+03	.454527E+01	.869034E+03	.634751E+01	.622290E+03
.102000E+03	.452916E+01	.872126E+03	.632501E+01	.624504E+03
.103000E+03	.451166E+01	.875507E+03	.630058E+01	.626925E+03
.104000E+03	.449280E+01	.879183E+03	.627423E+01	.629558E+03
.105000E+03	.447256E+01	.883161E+03	.624506E+01	.632406E+03
.106000E+03	.445097E+01	.887446E+03	.621582E+01	.635475E+03

Table 7 (Cont.)

.107000E+03	.442801E+01	.892046E+03	.618376E+01	.638769E+03
.108000E+03	.440371E+01	.896969E+03	.614982E+01	.642294E+03
.109000E+03	.437807E+01	.902223E+03	.611401E+01	.646056E+03
.110000E+03	.435109E+01	.907816E+03	.607634E+01	.650061E+03
.111000E+03	.432279E+01	.913760E+03	.603682E+01	.654317E+03
.112000E+03	.429317E+01	.920064E+03	.599545E+01	.658831E+03
.113000E+03	.426225E+01	.926740E+03	.595227E+01	.663612E+03
.114000E+03	.423002E+01	.933800E+03	.590726E+01	.668667E+03
.115000E+03	.419651E+01	.941257E+03	.586046E+01	.674007E+03
.116000E+03	.416172E+01	.949126E+03	.581187E+01	.679642E+03
.117000E+03	.412566E+01	.957422E+03	.576152E+01	.685582E+03
.118000E+03	.408834E+01	.966161E+03	.470940E+01	.691840E+03
.119000E+03	.404978E+01	.975360E+03	.565555E+01	.698427E+03
.120000E+03	.400998E+01	.985040E+03	.559998E+01	.705359E+03
.121000E+03	.396897E+01	.995219E+03	.554270E+01	.712648E+03
.122000E+03	.392674E+01	.100592E+04	.548373E+01	.720311E+03
.123000E+03	.388332E+01	.101716E+04	.542309E+01	.728366E+03
.124000E+03	.383872E+01	.102898E+04	.536080E+01	.736829E+03
.125000E+03	.379294E+01	.104140E+04	.529688E+01	.745721E+03
.126000E+03	.374601E+01	.105445E+04	.523134E+01	.755063E+03
.127000E+03	.369794E+01	.106816E+04	.516421E+01	.764879E+03
.128000E+03	.364875E+01	.108256E+04	.509551E+01	.775192E+03
.129000E+03	.359844E+01	.109769E+04	.502525E+01	.786029E+03
.130000E+03	.354703E+01	.111360E+04	.495346E+01	.797420E+03
.131000E+03	.349455E+01	.113033E+04	.488017E+01	.809397E+03
.132000E+03	.344100E+01	.114792E+04	.480539E+01	.821993E+03
.133000E+03	.338640E+01	.116642E+04	.472914E+01	.835246E+03
.134000E+03	.333077E+01	.118590E+04	.465145E+01	.849195E+03
.135000E+03	.327413E+01	.120642E+04	.457235E+01	.863887E+03

APPENDIX III

Hazards Analysis for Use of Neutron Diffraction Equipment at UMR Reactor*

Areas considered and solutions proposed:

I. Neutrons

The nature of the experiments require that a beam of neutrons be brought into the experimental area from the reactor core. This will be accomplished by using the beam tube. When the equipment is in operation, a beam measuring 1" x 2" (maximum) will be open to the room. The flux in this beam will be on the order of 10^9 neutrons/cm^2/sec. Normally beam area would be reduced to about 1 cm^2 for operation.

About 1% of this beam would be reflected by Bragg plane reflection. These neutrons would normally be completely stopped by the detector shield. If the experiment is such that the detector is not in the primary reflected beam, special shielding will have to be provided.

The dose rate one foot from the LiF crystal due to non-coherent scattering (reflected beam not included) would be about 0.040 rem/hr.

The remainder of the beam would travel to the beam catcher, where it should be completely absorbed. This beam catcher is constructed from borated paraffin (.15 lb. boric acid per lb. paraffin min.). The thickness in the primary beam is approximately 9 inches. A sheet of cadmium has been placed behind the paraffin.

The neutron beam will cause activation of the air in the beam tube and in the experimental area. It is proposed that the beam tube be sealed by a thin aluminum plate placed at the front of the stationary portion of the plug. This would keep the radioactive gases from escaping into the room.

*As presented to the Reactor Safety Committee on March 9, 1965.

The activity of the air in the room would be approximately 0.079×10^{-6} μc/ml. This assumes that the A^{41} produced in the beam, after the beam leaves the beam tube, is dispersed evenly throughout the entire room.

The maximum permissible concentration of A^{41} permitted in a restricted area is 2×10^{-6} μc/ml (Appendix B, Table 1, Part 20, Title 10, AEC Regulations).

A shielding plug is proposed that would have a front section that would revolve to effectively close the beam tube passage when the equipment is not in operation.

This revolving plug would have Boral end plates which would be black to thermal neutrons. This should reduce the neutron beam to normal working levels, that is less than 2 mr/hr. The front Boral plate should also reduce activation of the concrete in the plug.

II. Gamma

The gamma intensity in the beam tube has been measured to be of the order of 2×10^3 r/hr.

It is proposed that a lead gamma shield be placed in front of the beam tube collimator plug. Two inches of lead in this position should cause few problems with the neutron beam and should reduce the gamma to approximately 1.88×10^2 r/hr.

Some scattering will occur in the crystal and in the beam catcher. This will, in both cases, be less than 2 mr/hr at one foot from the crystal or beam catcher.

The beam of gamma will be dissipated by the concrete wall. The scattering from the wall will be less than 2 mr/hr at one foot from the wall.

General Considerations:

A monitor for gamma radiation is already present in the beam room. This gives an annunciation and a rundown when the level exceeds 10 mr/hr.

It is proposed that a neutron monitor also be installed. The master unit for this would be installed in the control room and a warning device installed that would give an indication of a high neutron level in the experimental area.

It is also proposed that the rotating portion of the shield plug be interlocked to give an annunciation when the plug is not in its fully closed position. It is further proposed that a rotating red beacon be installed which would automatically come on when the revolving plug is not fully closed.

Calculation of Activation of Gases in Beam Tube and Possible Release:

Assume 6" diameter 10 feet long (this would be maximum possible volume)

D = 6"   r = 3" = 7.62 cm

L = 10'   = 120" = 305 cm

$V = \pi r^2 L$

$V = \pi(7.62)^2(305)$

$V = 5.57 \times 10^4\ cm^3$

V = 55.7 liters

one mole = 22.41

V = 2.48 moles

$N = 1.5 \times 10^{24}$ atoms

A^{41}

$A_\infty = N\sigma\phi$

$A_\infty = (1.5 \times 10^{24})\ (9.4 \times 10^{-3})\ (0.53 \times 10^{-24})\ (10^9)$

$A_\infty = 7.49 \times 10^6$

$$C = \frac{7.49 \times 10^6}{3.7 \times 10^{10}} = 2.02 \times 10^{-4} \text{ curies}$$

$$C = 0.202 \text{ m c of } A^{41}$$

if N is used as a purge

$$A_\infty = N\sigma\phi$$

$$A_\infty = (1.5 \times 10^{24})\ (3.7 \times 10^{-3})\ (30 \times 10^{-6})\ (10^{-24})\ (10^9)$$

$$A_\infty = 1.66 \times 10^2$$

$$C = \frac{1.66 \times 10^2}{3.7 \times 10^{10}}$$

$$C = 4.5 \times 10^{-9} \text{ curies}$$

$$C = 0.0045\ \mu c$$

Activity Induced in the Air in the Experimental Area:

1. Assume maximum beam of 2 in^2

2. Assume beam catcher 8' from beam port total volume of air exposed to beam

$$V = (A)\ (L)$$

$$V = (2.54)\ (5.08)\ (96)\ (2.54)$$

$$V = 3.15 \times 10^3$$

$$V = 3.15 \text{ liters}$$

$$V = \frac{3.15}{22.4}$$

$$V = 0.141 \text{ moles}$$

$$N = 0.141 \times 6.02 \times 10^{23}$$

$$N = 8.45 \times 10^{22} \text{ atoms}$$

Activity Due to A^{41} Production:

$$A_{\infty} = N\sigma\phi$$

$$A_{\infty} = (8.45 \times 10^{22}) (9.4 \times 10^{-3}) (0.53 \times 10^{-24}) (10^{9})$$

$$A_{\infty} = 42.2 \times 10^{4}$$

$$C = \frac{4.22 \times 10^{5}}{3.7 \times 10^{10}}$$

$C = 1.14 \times 10^{-5}$ curies

Assume this will be dispersed over entire volume of air in room (approximately 15' x 34' x 10')

$V = 1.44 \times 10^{5}$ liters

$$S = \frac{1.14 \times 10^{-5}}{1.44 \times 10^{5}}$$

$S = .79 \times 10^{-10}$ curies/liter

$S = 0.079 \times 10^{-6}$ μc/ml

Non-Coherent Neutron Scatter From LiF Crystal:

Neutron remaining after passing through material

$$N = N_0 e^{-\Sigma_s t}$$

$$N = 10^{9} e^{-0.065(2)}$$

$$N = 8.78 \times 10^{8}$$

or total scattered $= 1.22 \times 10^{8}$

Assume isotropic scatter flux at 30 cm (approximately 1')

$$A = 4\pi r^{2}$$

$$A = 1.13 \times 10^{4}$$

$$\phi = \frac{1.22 \times 10^{8}}{1.13 \times 10^{4}}$$

$\phi = 1.08 \times 10^{4}$ neutrons/cm^{2}/sec

2.7×10^{5} neutrons/cm^{2}/sec = 1 rem/hr dose rate at 30 cm $= \frac{1.08 \times 10^4}{2.70 \times 10^5} = 0.040$ rem/hr

Gamma Attenuation by 5 cm of Lead:

(Proposed gamma shield in beam tube in front of collimator)

$I = I_0 e^{-\mu x}$

Assume minimum value for

$I_0 = 2 \times 10^3$ r/hr

$I = I_0 e^{-0.475(5)}$

$I = 2 \times 10^3 e^{-2.37}$

$I = 1.88 \times 10^2$ r/hr

Reduction of Gamma by Shielding Plug:

Using barytes concrete front plug 50 cm long

$I = I_0 e^{-\mu x}$

$I = 1.88 \times 10^2 e^{-0.109(50)}$

$I = 1.88 \times 10^2 e^{-5.45}$

$I = 0.81$ r/hr

Gamma Scatter by LiF Crystal:

$I = I_0 e^{-\mu x}$

$I = 1.88 (\times 10^2) e^{-0.03(1)}$

$I = 1.83 \times 10^2$

Gamma scattered = 5 r/hr

Assume isotropic scatter at 1' from crystal

$A = 1.13 \times 10^4$

$D = \frac{5}{1.13} \times 10^{-4}$

$D = 4.4 \times 10^{-4}$ r/hr

Dose rate at one foot from crystal L/mr

Scatter of Gamma from Concrete Wall:

area of beam = 4 x 5 cm = 20 cm^2

$\frac{\sigma}{\rho} = N \frac{Z}{A} e6$

$\frac{\sigma}{\rho} = \frac{0.623 \times 10^{24}}{2} (1/2) (0.04 \times 10^{-24})$

$\frac{\sigma}{\rho} = .00602$

$\sigma = .014$

Assume scatter of interest occurs in 1st cm of concrete

I = unscattered gamma radiation

$I = I_0 e^{-\mu x}$

$I = 1.88 \times 10^2 \; e^{-.014}$

$I = 1.88 \times 10^2 \; (.95)$

$I = 1.78 \times 10^2$

I scattered = 10 r/hr

Assume isotropic scatter at 1' from surface

$A = 0.56 \times 10^4$

$D = \frac{10}{5.6 \times 10^3} = 1.78 \times 10^{-3}$ r/hr = 1.78 mr/hr

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