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Digital Controller for Stepping Motor-Driven X-ray Diffractometer

by

P.C. Naval, Jr., P.P. Saligan,
& V.B. Soriano-Calix*

ABSTRACT

Presented is a stepping motor controller for the Philips PW 1050 Vertical Goniometer featuring crystal-controlled scan rates of 4, 2, 1, 1/2, 1/4, and 1/8 degrees per minute in the continuous scan mode, and step sizes of 0.005, 0.01, 0.02, 0.025, 0.05, 0.1, 0.2, and 0.5 degree when operated in the step scan mode. A slew rate of 96 degrees per minute is provided for positioning purposes.

The TTL-implemented design accommodates upgrading to higher levels of automation by a simple substitution of the control logic section.

INTRODUCTION

X-ray diffraction exploits the fact that atoms in crystalline solids are arranged in three dimensionally recurring lattices which act as a diffraction grating to cause scattering of incident x-rays. W.L. Bragg has shown that these waves will constructively reinforce one another if they are in phase, with paths differing by an integral number of wavelengths to satisfy the relation $2\ d \sin \theta = n\lambda$ where d is the interplanar spacing, λ the x-ray wavelength, θ the angle of incidence, and n an integer. When a sample is irradiated with x-rays, they are diffracted according to the characteristics of the compounds present. By measuring the angles at which diffraction peaks occur and their intensities, information on the sample's crystal structure may be inferred.

A stepping motor-driven Philips PW 1050 Vertical Goniometer was acquired with the intention of obtaining the accompanying motor control unit. Restrictions on purchases involving foreign currency prompted the fabrication of the needed motor controller. This work describes a controller capable of driving the goniometer in both continuous and step scan modes at different scanning rates and step sizes.

In the continuous scanning mode the goniometer arm moves in 0.005 degree increments at the selected rate. Speeds of 4, 2, 1, 1/2, 1/4, and 1/8 degrees per minute are possible together with a slew rate of 96 degrees per minute needed to position the arm at the angle desired. The goniometer operated in this mode, and used in conjunction with a ratemeter and a chart recorder, permits quick and visual determination of the angular positions of peaks thereby allowing detailed scanning only around angles of interest.

Digital data may also be provided when the arm step-scans the sample. Step scanning involves incrementing the angular position by a selected angular step, collecting counts over a preset

*The authors are with the Physics Research Division of the Philippine Atomic Energy Commission, Diliman, Quezon City, Philippines.

time, recording the accumulated count, and advancing to the next position to start another cycle. Angle increments of 0.005, 0.01, 0.02, 0.025, 0.05, 0.1, 0.2, and 0.5 degree (2 theta) are available in this mode.

It is in the step scan mode that the controller adapts itself to higher levels of automation. In the basic system, a printer together with a scaler, controlled with pulses from the control logic, permits acquisition of data in digital form well suited for computer processing. In an automatic system, both scanning modes may be programmed, with the actual scanning procedure controlled by a microprocessor. Data from the scaler may be processed by filtering algorithms before dumping to a larger computer.

GENERAL DESCRIPTION

It is the task of the Controller to move the goniometer arm at a desired speed in either increasing or decreasing scattering angle and to position the arm to any angular value within its range. This is done by controlling a permanent magnet stepping motor coupled to a worm drive mechanism which positions the arm at an angle 2θ (relative to the incident beam) and tilts a sample holder at half that angle. Stepping motors are driven by sequentially exciting the armature winding according to a certain order. Inverting the order reverses the direction of rotation. The motor's speed is controlled by varying the repetition frequency of the exciting pulses. Unlike most motors, steppers are easily interfaceable to digital controllers [1].

Four functional blocks comprise the Controller (Fig. 1). The Clock-Divider serves as a stable frequency source on which the accurate generation of scan rates is based. The Speed/Size Selecting Block receives instructions as to the Controller's mode of operation and scan speed or step size through its MODE and SELECT inputs. When continuous scanning is chosen, this block generates a continuous pulse train of definite frequency which translates to goniometer arm motion of constant speed. This is done by successive frequency division of the Clock-Divider output. A step scan increment may be seen as a gated pulse train, with the number of pulses in the envelope corresponding to the number of steps that the motor is to execute.

The output of the Speed/Size Selecting Block goes to the Translator which excites the motor winding in the proper sequence. This block also dictates the direction of rotation by changing the sequence order to effect increasing or decreasing angular motion. The Power Driver Block matches the logic level signals of the Translator with the high drive current requirement of the stepping motor and minimizes power drain by cutting off power to the motor when the shaft has reached its target position.

Within the Speed/Size Selecting Circuit are the Counter, Start/Stop Flip-flop, Speed Selector, Step/Size Decode, and Step/Size Selector sections. The Start/Stop Flip-flop controls the operation of the Counter, inhibiting the latter when set and enabling it when reset. This flip-flop accepts START and STOP pulses as inputs.

Initially, the Counter is disabled by the Start/Stop Flip-flop. Upon reception of an external START pulse, this flip-flop allows the Counter to count the pulses from the Clock-Divider. In the continuous scan mode, the Counter functions as a divider which generates the seven frequencies corresponding to the seven detector slew and scan rates. The eighth speed comes from the EXT IN input which may be driven by an external oscillator at the rate desired. The outputs of this divider are taken as inputs by the Speed Selector. Through the select input lines, one of these inputs is allowed to clock the Translator. As soon as the STOP pulse is received, the flip-flop is reset, extinguishing the clocking pulses to the Translator.

For step scan operation, an external START pulse sets the Counter running. As the Counter increments, its outputs are being decoded by the Step/Size Decode section, for states corresponding to step sizes of 0.005, 0.01, 0.02, 0.025, 0.05, 0.1, 0.2, and 0.5 degree and the decoded outputs are taken in by the Step/Size Selector. The desired step size is chosen through the select input lines. The selected Step/Size Decode output goes active upon decoding the right number of steps and resets the Start/Stop Flip-flop. Effectively, the pulse train is gated, moving the detector arm by a chosen angular increment.

A stepping motor contains a number of stator windings into which driving pulses may be applied. Shaft rotation results from exciting the different sets of windings in a sequence. The Translator Block converts the serial pulse train output of the Step/Size Selecting Circuit into this sequence of winding excitation pulses. The Counter-Decoder section counts the input pulses, decodes the counts, and asserts one of the four possible outputs which, after buffering, will drive the stepping motor windings. At a particular position, the motor shaft can turn in either direction depending on which neighboring winding is excited next. The Direction Flip-flop within the Translator determines which.

The Power Driver Block delivers the required current into the motor and cuts off power to the winding when the shaft has already reached its target position. The Driver section provides the power amplification for proper excitation of the windings by the Translator outputs.

Even when the windings are not energized, the permanent magnet stepping motor possesses an inherent holding torque which holds the rotor in place [2], eliminating the need to excite the coils at standstill. The Power Driver capitalizes on this characteristic by energizing the windings only when the motor steps to the next position. Cutting off power to the motor is possible because of the TTL-Controlled Power Supply section. A Negative Recovery Circuit [3] in this block prolongs the last applied pulse to keep the rotor from overshooting the intended position.

CIRCUIT DESCRIPTION

The Clock-Divider

The CMOS gate ICIA together with the 1.0 MHz crystal XTAL1, generates precise square waves [4] for frequency division by MSI counters IC3, IC4, and IC5. Counter IC3 functions as a modulo-13 or modulo-2 counter when the FAST input is low or high respectively. IC4 and IC5 further divide the frequency by 120. The 1.0 MHz output of IC2 is divided by 1560 (FAST=0) or 240 (FAST=1) for input to the next block. The 1.0 MHz clock is also available through the CLOCK 1 output.

The Speed/Size Selecting Circuit

MSI counters IC6, IC7, and IC8 comprise the Counter section of this Block (see Fig. 3). When enabled, the Counter generates the following frequencies: 320, 13 1/3, 6 2/3, 3 1/3, 1 2/3, 5/6, and 5/12 Hz, through the outputs of IC6, IC7, and IC8. These frequencies, corresponding to the scan rates of 96, 4, 2, 1, 1/2, 1/4, and 1/8 degrees per minute, are the inputs to the Speed Selector IC9. Through IC9's select inputs, one of these inputs is passed to selector IC13. If continuous scan mode is chosen, this signal is allowed to clock the Translator.

Start/Stop Flip-flop IC14A controls the operation of the Counter via $\overline{Q}$ output. In the reset state, IC6, IC7 and IC8 are all inhibited. When a START pulse is received by IC14A, the Counter is permitted to count the clocking pulses from the previous block.

AND gates within IC11 and IC12 form the Step/Size Decode section. In choosing the step scanning mode, selector IC13 allows pulses from the Q_A output of IC7 to reach the Translator. The Step/Size Decode gates were wired so that one of the eight go active when the state corresponding to the eight different step sizes is reached. One of these states is chosen through Step/Size Selector IC10 which resets the Start/Stop Flip-flop as soon as the selected step increment is executed. The Counter's state is initialized to zero when disabled. Half of IC15 was used as a power up reset generator. The output of this circuit clears IC14A on power up.

The Translator

A 74LS191 up/down counter and a 74LS139 decoder comprise the Counter-Decoder. The output pulses from the previous block are counted by IC16. Two bits from the counter output serve as an address to any of the four outputs of IC17 that will be asserted. Since the counts of IC16 are consecutive, the outputs of IC17 will be the sequential outputs needed by the windings. IC18A to D act as buffers for driving the transistor switches of the next block which require a higher voltage swing for proper operation. Direction Flip-flop IC14B dictates the order of the sequence by controlling the count direction (count up or count down) of IC16. When IC14B is reset, outputs are asserted in an A-B-C-D fashion, which translates to an increasing angle motion. A D-C-B-A order of excitation reverses the direction of motion.

The Power Driver

This Block, consisting of transistor switches Q6, Q7, Q8, and Q9 (see Fig. 5), matches the buffered outputs of the Translator with the high current demand of the motor windings. Diodes D2, D3, D4, and D5 suppress the high inductive kick of the windings while resistance R17 limits the maximum current into the motor. Q4 and Q5 allow the motor power supply to be under the control of the Negative Recovery Circuit (see lower right corner of Fig. 3). This circuit is a retriggerable monostable which stays on as long as the Translator clock pulses keep arriving below the rate defined by R3 and C3. When the last pulse is received, the circuit goes low after the duration R3C3. This extends the last energizing pulse for that duration thereby forcing the rotor to stay in the target position.

The Control Logic

This section allows the user to control the operation of the Controller via pushbutton switches and displays such information as the mode of operation, speed or step size and scan direction.

The MODE selector circuit (Fig. 6a) consists of a toggle flip-flop IC20A clocked by a switch debouncer. When the MODE switch S1 is pressed, the debouncer output goes low until the switch is released [4]. IC20A toggles on the negative-going output of the debouncer. The output of IC20A goes to the MODE control input of the Speed/Size Selecting Circuit. When step scanning, the motion of the motor may be speeded up by connecting this output to the FAST input of the Clock-Divider (Fig. 1). The Controller's operational mode is known through LEDs D14 and D15 labelled STEP SCAN and CONT SCAN respectively (see Fig. 7b).

The debounced output of SELECT switch S2 clocks counter IC22 which furnishes inputs to the Speed/Step Size Selectors IC9 and IC10 (Fig. 3). IC21 decodes this input word and lights the appropriate LED to indicate the selected speed or step size. LEDs D6, D7, D8, D9, D10, D11, D12 and D13 are labelled SLEW 4, 2, 1, 1/2, 1/4, 1/8 and EXT two theta degrees per minute and 0.005, 0.01, 0.02, 0.025, 0.05, 0.1, 0.2, and 0.5 two theta degree, respectively. The RUN output into the ENABLE input prevents changes in the speed/step size setting when the motor is running. When a power up reset is generated, the CLEAR input initializes IC22 and the BLANK input blanks all of D6 to D13 informing the user that the system is being reset.

Scan direction control is provided by the switch debouncing circuit (Fig. 6c) which toggles Direction Flip-flop IC14B (Fig. 4). High and low angle limit switches are directly connected to the corresponding inputs of IC14B.

Motor start and stop control is achieved by the circuits shown in Fig. 7a and 7b. And-Or-Invert IC24 functions as a selector that controls which START inputs are to reach Start/Stop Flip-flop IC14A. When step scanning (MODE = 1), S4 is disabled to give way to a START signal of external origin. Stop switch S6 furnishes a STOP signal to IC14A when activated. The reset signal, produced by pressing S5, initializes the state of the system.

Information on the operational mode and scan direction are provided by LEDs D14 to D17. MODE and UP/DN levels light up the appropriate indicators through drivers Q10 to Q13 (Fig. 7b).

THE BASIC XRD SYSTEM

A simple manually operated XRD system with capability of providing data in both analog and digital form is described. The system consists of nuclear instrumentation modules available in the laboratories of PAEC. System configuration is shown in Figure 8.

The high voltage supply furnishes the 1.5 KV operating bias for a xenon-filled proportional detector which includes a preamplifier in a compact enclosure. The LLD and Window discrimination settings of the Amplifier and Single Channel Analyzer were adjusted for proper Cu K-beta rejection. Rewiring of the amplifier's connector was done to make it compatible with the detector's pin assignments. The output of the Amplifier and SCA is fed to the Linear Ratemeter and to the Scaler.

The Linear Ratemeter has a standard deviation selector which gives the maximum full scale statistical fluctuation expressed as a percentage of final steady state value [5]. In our experiments, the one percent setting gave us smooth plots without sacrificing peak definition. A recording of the scattered intensity versus detector position (2 theta) is obtained using an HP 7101B or Varian A-25 Chart Recorder. Chart speed is selected to synchronize with the diffractometer scan rate. Performance tests were done using a silicon standard sample. The diffraction pattern obtained using the nickel-filtered copper radiation was comparable to the published pattern acquired using commercial diffractometers. The accuracy was determined by using the 311 reflection of powdered silicon. The measured position was less than 0.02 degree from the theoretical value. Figure 9 shows a diffractogram of the standard obtained at the scan rate of 2 degrees (2θ)/ minute. The expanded portion of the 311 reflection taken at 1/4 degree (2θ)/minute is in Fig. 10.

Intensities may be recorded in numeric form when the system step-scans. The arm is first positioned to the desired angle and the desired count time entered through the thumbwheel switches of the Timer with the Count/Stop switch set to STOP. The process is initiated by flipping this switch to Count. This permits both the Counter and Timer to count. When the preset time is reached, the Timer issues a STOP pulse which instructs the Line Printer to print the contents of the Counter's registers and informs the controller to move the arm to the next position. As soon as the printer has recorded the contents of the scaler, a reset is generated which starts a new cycle. Through the Recyle Control input, the Controller inhibits the Line Printer from generating this reset when the arm has not yet reached its intended angular position. The process is manually terminated once the angles of interest have been scanned. Figure 11 shows an intensity-vs-angle plot of the 311 reflection obtained in the step scan mode.

CONCLUSION

The system just described is highly flexible, as the modules can be arranged to suit the particular needs of the investigator. Configured in another way, the system can record the integrated intensities of peaks, with minimum operator intervention. The choice of module is not critical, for similar modules in place of the ones named will make the system work as well, as long as the logic of operation of the system is respected.

For more than six months now, the diffractometer system has been in use for phase and structure analyses of beta-alumina compounds and magnetic oxides in the studies undertaken by the group.

With minor changes in the design, the digital controller may be adapted in neutron scattering and angular correlation set-ups.

ACKNOWLEDGMENT

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SPECIFICATIONS

Required Power Source:
- Logic: 5V, 2A Regulated
- Motor: 12V ± 10%, 3A

Time Base Clock Rate: 1.00 MHz

External Functions:
- START, STOP, MODE, SELECT, EXT IN, SCAN DIR, RESET

Stepping Mode: Full-Step, Unipolar, One Winding on

Continuous Scan:
- Goniometer Scan Rates:
  - 96 (slew), 4, 2, 1, 1/2, 1/4, 1/8 degrees per minute and EXT input for variable scan rate.

Step Scan:
- Goniometer Step Sizes:
  - 0.005, 0.01, 0.02, 0.025, 0.05, 0.1, 0.2, and 0.5 degree (2 theta)

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[3] H.M. BERLIN, The 555 Timer Applications Sourcebook. Derby, Conn.: E & L Instruments, Inc. 1976, pp. 2.6-2.8.

[4] D. LANCASTER, TTL Cookbook, Indianapolis: Howard Sams & Co., 1976, pp. 169-170.

[5] ORTEC Model 441 Ratemeter Operating and Service Manual.

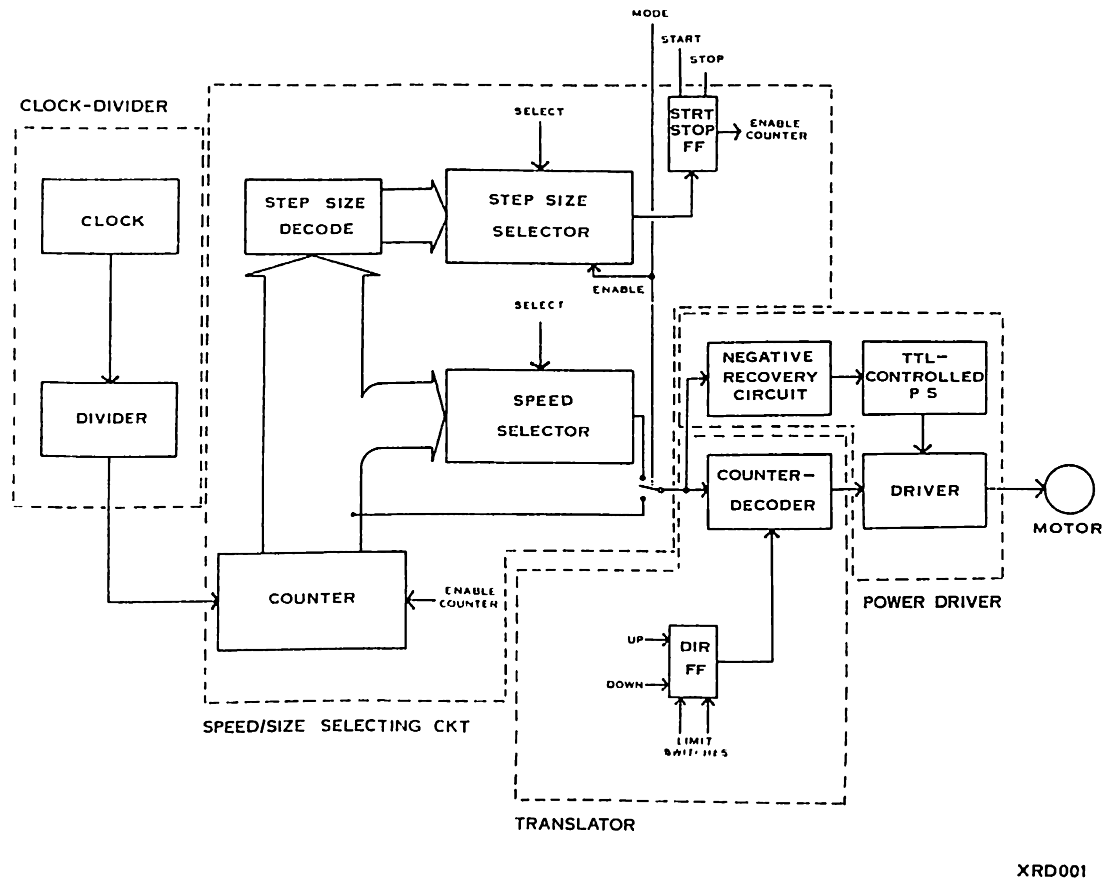

Figure 1. Block Diagram of the Controller.

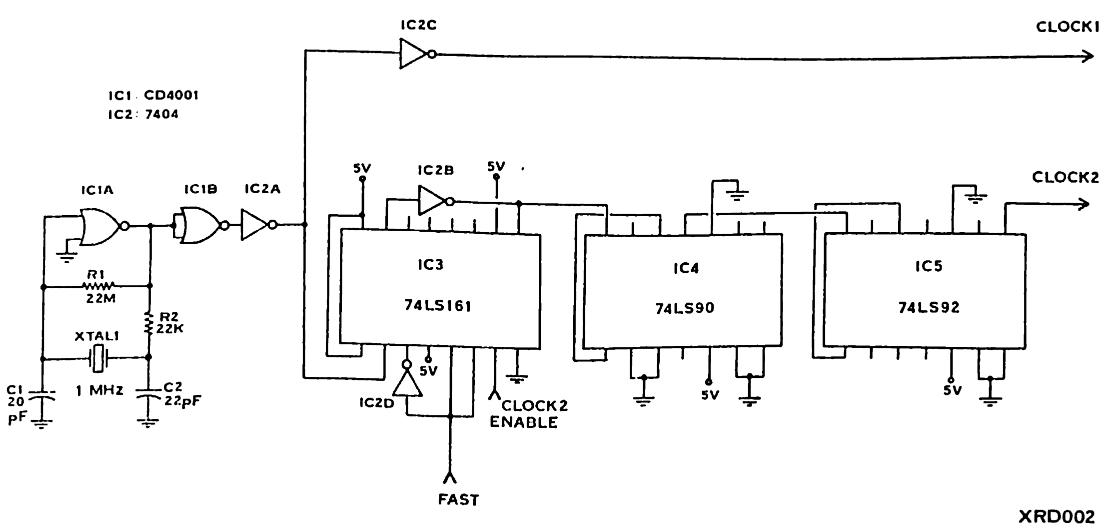

Figure 2. The Clock-Divider Circuit.

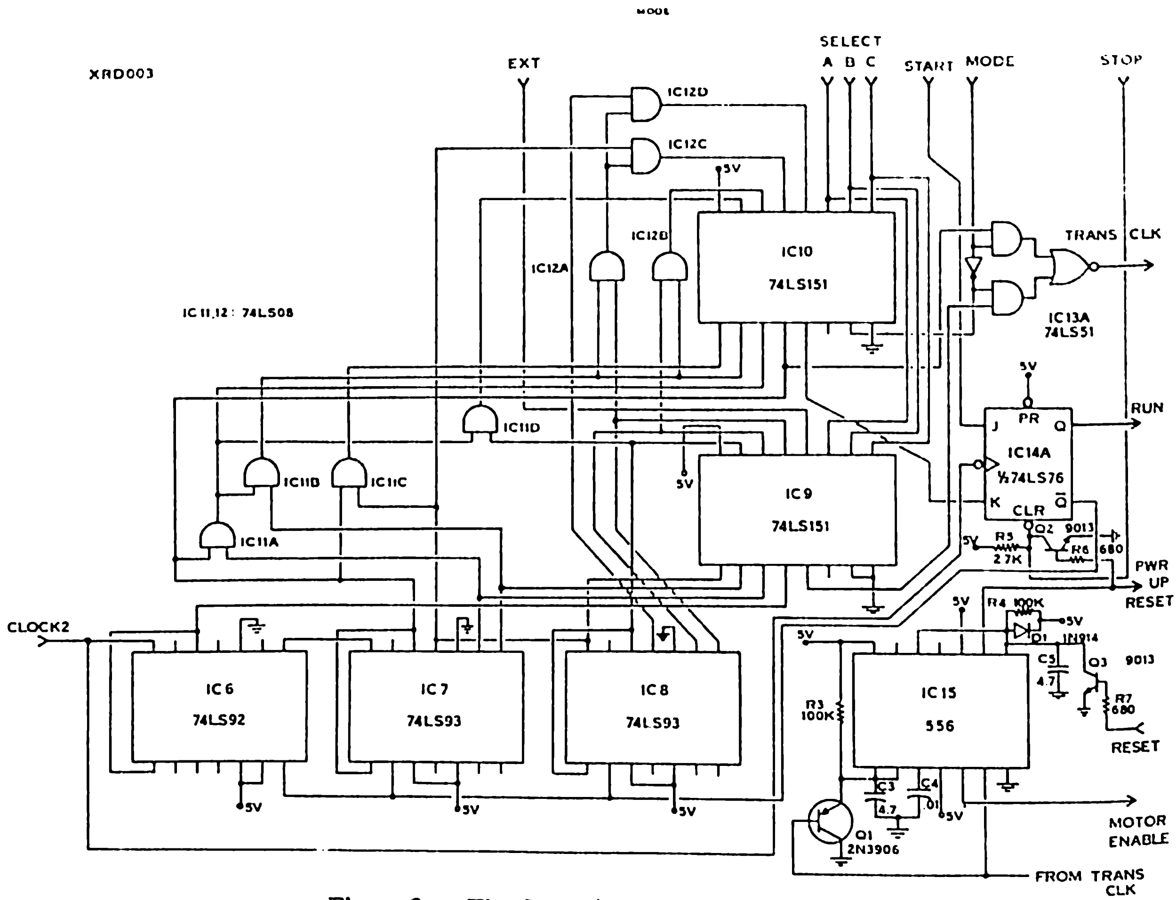

Figure 3. The Speed/Size Selecting Circuit.

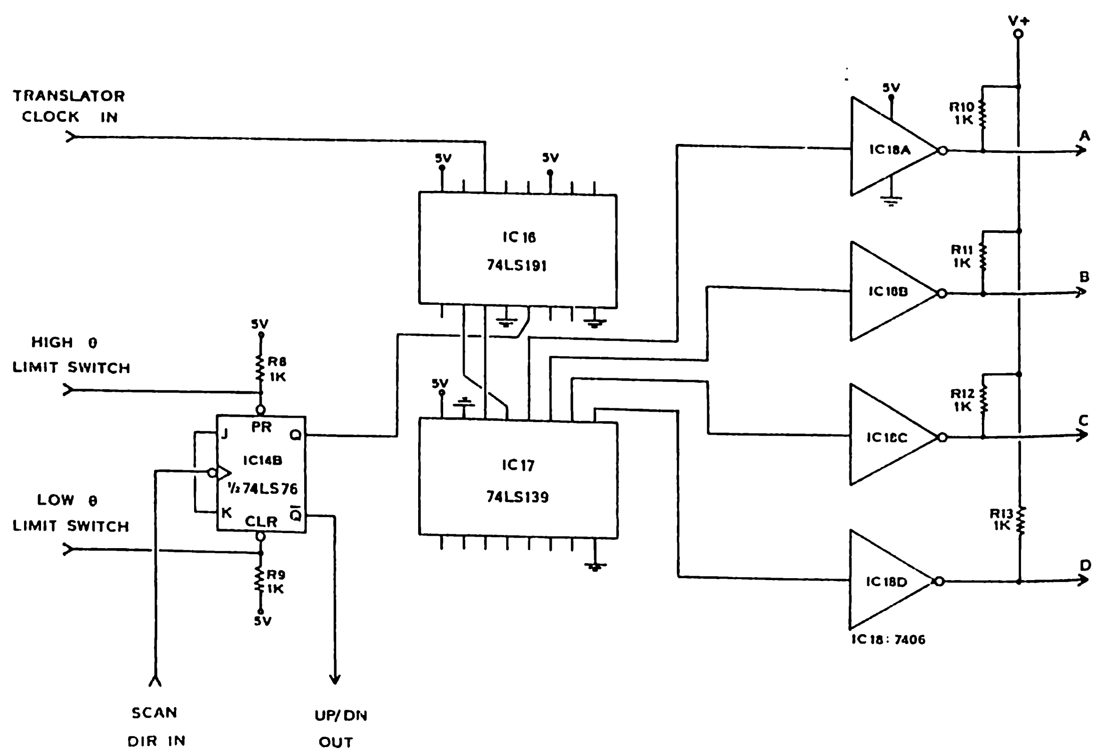

Figure 4. The Translator Circuit.

XRD004

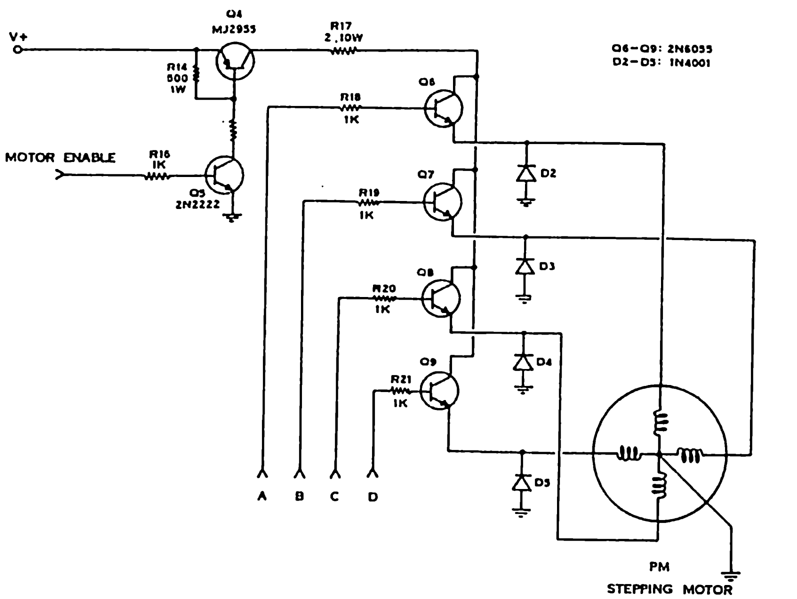

Figure 5. The Power Driver. XRD005

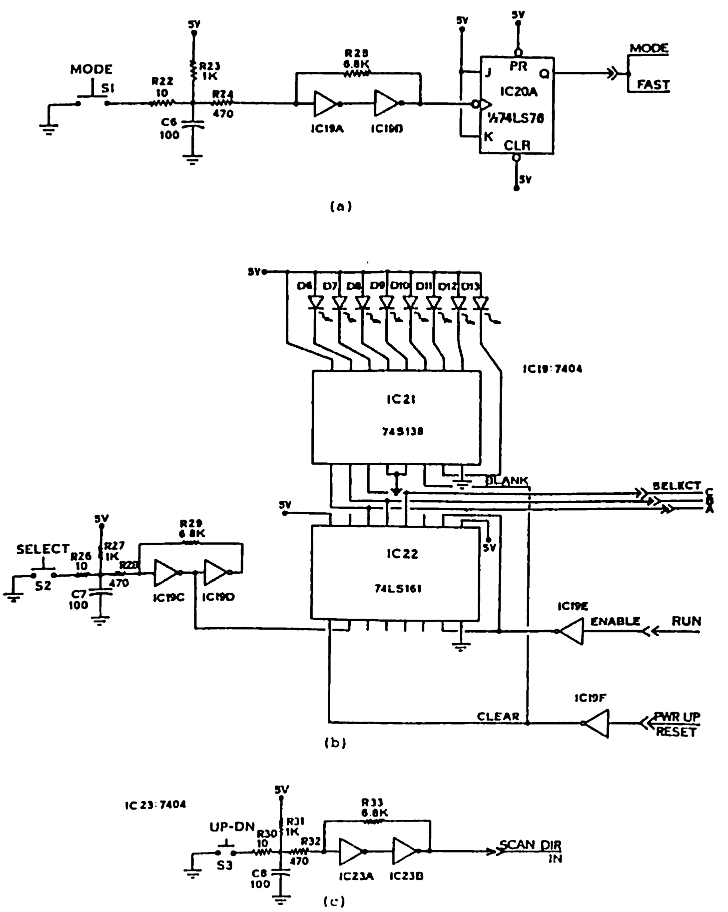

Figure 6. A Portion of the Control Logic. XRD006

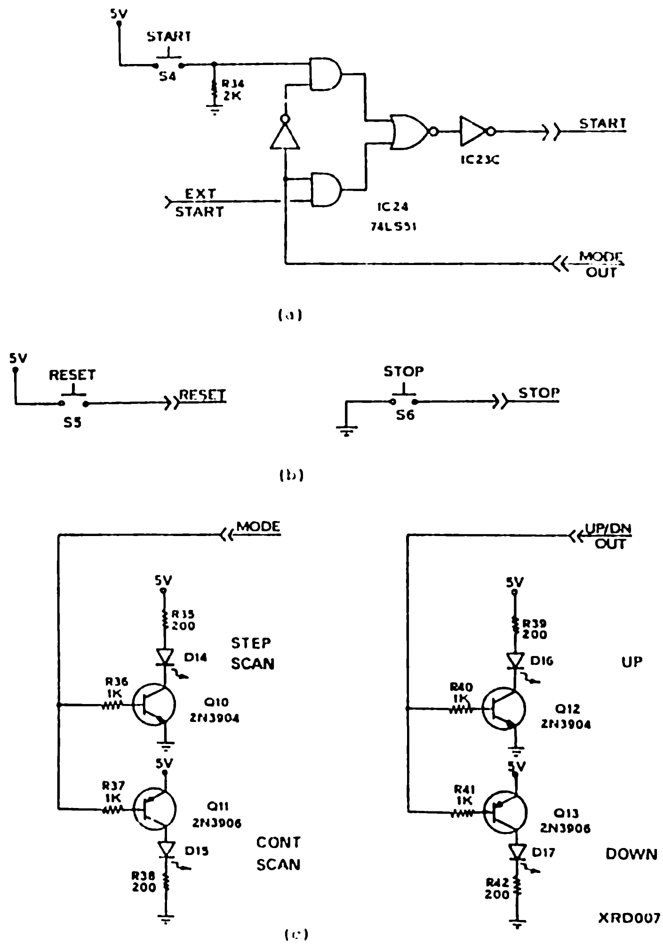

Figure 7. Part of the Control Logic.

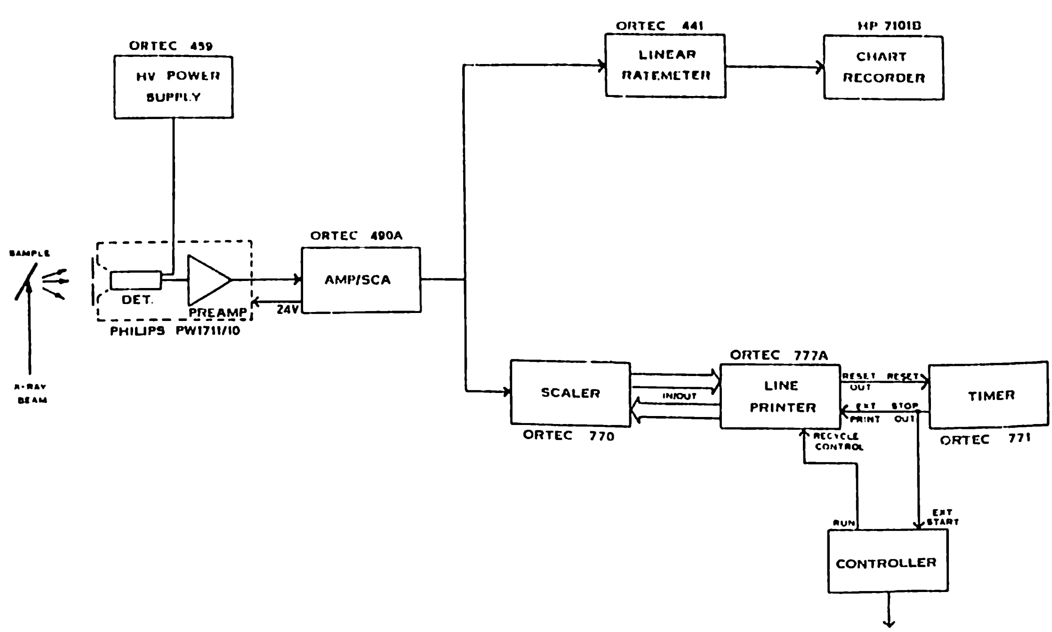

Figure 8. Block Diagram of the Basic XRD System.

XRD008

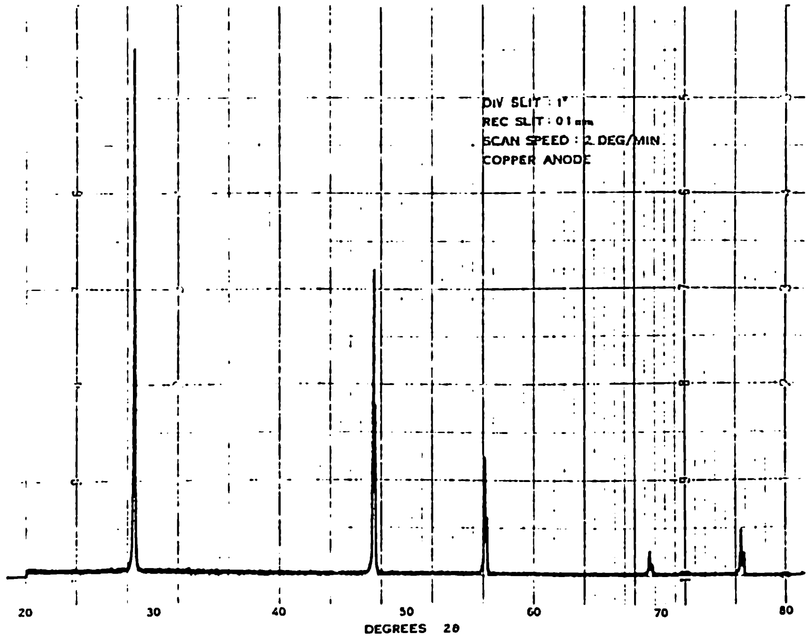

Figure 9. Diffractogram of Silicon Powder Using Our XRD System.

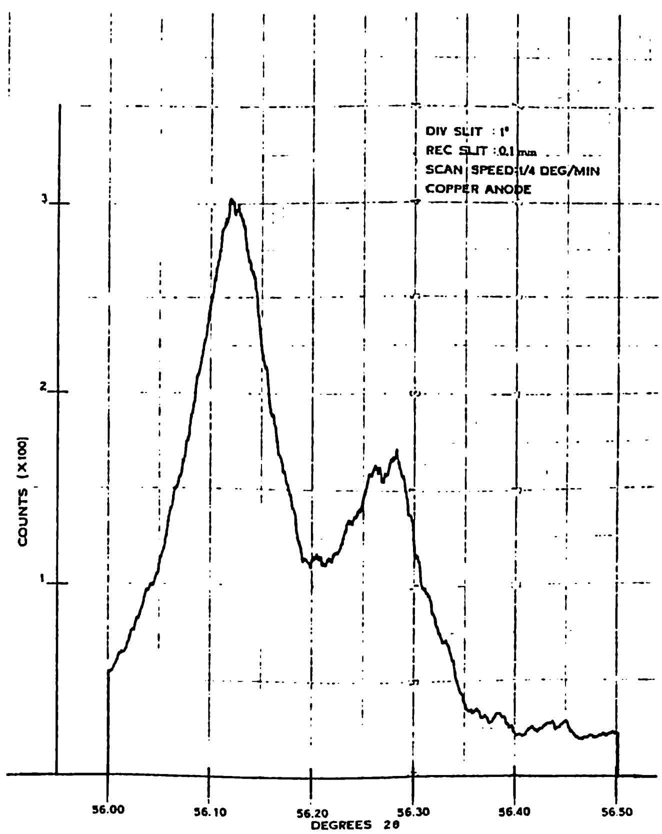

Figure 10. Diffractogram of the (311) Reflection of Silicon Powder at 56.12°

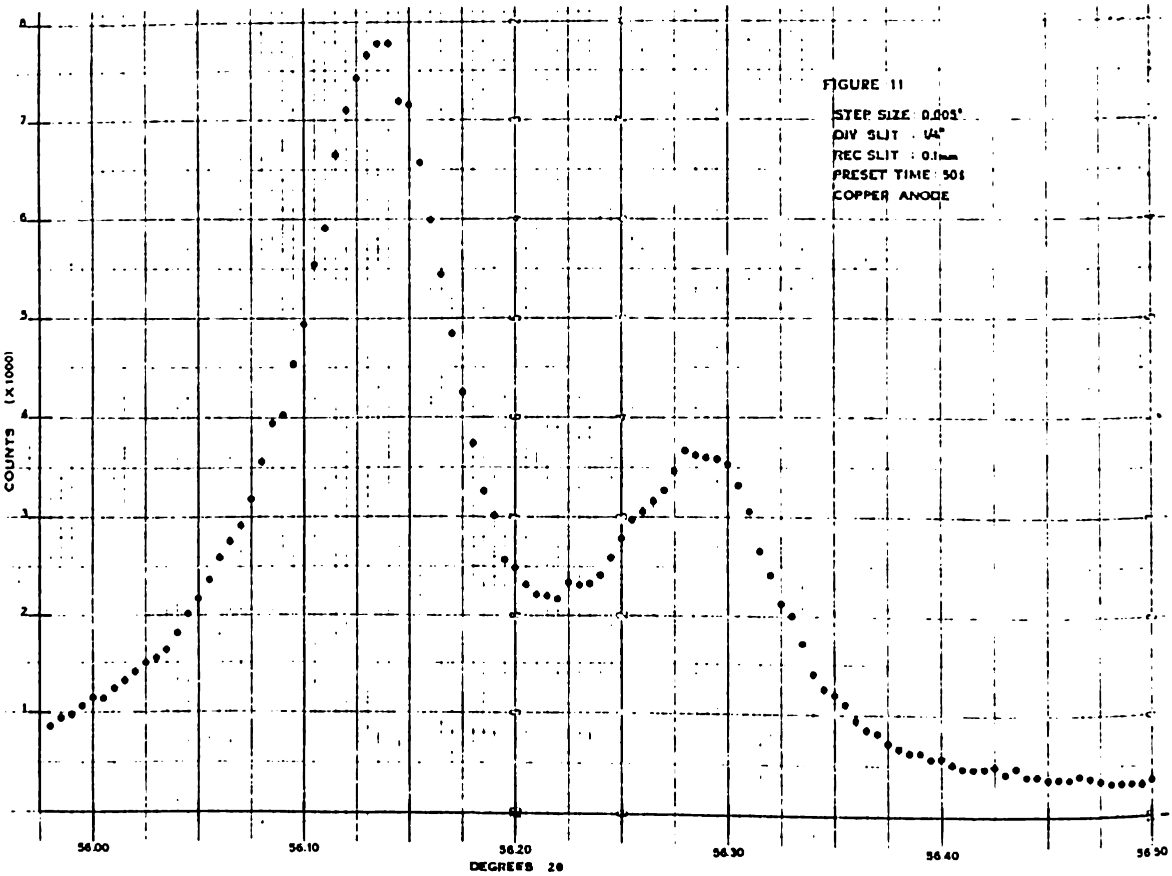

Figure 11. Intensity vs. Angle Plot of the 311 Reflection