Motorized Beam Alignment of a Commercial X-ray Diffractometer

Noah R. Van Zandt and James F. Myers
Cedarville University, Cedarville, Ohio

Richard B. Rogers
Glenn Research Center, Cleveland, Ohio
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National Aeronautics and Space Administration

Glenn Research Center
Cleveland, Ohio 44135

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Cedarville University
Cedarville, Ohio 45314

Richard B. Rogers
National Aeronautics and Space Administration
Glenn Research Center
Cleveland, Ohio 44135

Abstract

X-ray diffraction (XRD) is a powerful analysis method that allows researchers to noninvasively probe the crystalline structure of a material. This includes the ability to determine the crystalline phases present, quantify surface residual stresses, and measure the distribution of crystallographic orientations. The Structures and Materials Division at the NASA Glenn Research Center (GRC) heavily uses the on-site XRD lab to characterize advanced metal alloys, ceramics, and polymers.

One of the x-ray diffractometers in the XRD lab (Bruker D8 Discover) uses three different x-ray tubes (Cu, Cr, and Mn) for optimal performance over numerous material types and various experimental techniques. This requires that the tubes be switched out and aligned between experiments. This alignment maximizes the x-ray tube's output through an iterative process involving four set screws. However, the output of the x-ray tube cannot be monitored during the adjustment process due to standard radiation safety engineering controls that prevent exposure to the x-ray beam when the diffractometer doors are open. Therefore, the adjustment process is a very tedious series of blind adjustments, each followed by measurement of the output beam using a PIN diode after the enclosure doors are shut. This process can take up to 4 hr to perform.

This technical memorandum documents an in-house project to motorize this alignment process. Unlike a human, motors are not harmed by x-ray radiation of the energy range used in this instrument. Therefore, using motors to adjust the set screws will allow the researcher to monitor the x-ray tube’s output while making interactive adjustments from outside the diffractometer. The motorized alignment system consists of four motors, a motor controller, and a hand-held user interface module. Our goal was to reduce the alignment time to less than 30 min. The time available was the 10-week span of the Lewis' Educational and Research Collaborative Internship Project (LERCIP) summer internship program and the budget goal was $1200. In this report, we will describe our motorization design and discuss the results of its implementation.

Overview

The motorized alignment system consists of three major components: the gear motors, the main electronics unit, and the hand-held controller (Fig. 1). The gear motors are simply four brushed gear motors, one for each of the adjustment screws on the x-ray tube. The main electronics unit contains all of the major system electronics including the power supply, motor controller, and relays. Finally, the handheld controller contains the necessary switches and knobs to interface the user with the system. Additionally, the circuit schematic can be found in the Appendix. Table 1 shows motor nomenclature and adjustment functions.

Full automation of the alignment process was also considered. However, the work needed to program a microcontroller and add emergency stops to prevent movement past physical limits would be a significant increase in complexity with marginal additional benefit if the goal of reducing alignment time to less than 30 min via remote manual control could be achieved.
**Motors**

We chose to use brushed dc motors because they are simpler and easier to control than other motor types. By also making the motors geared, we allowed the user to be able to fine tune much easier because of the motor’s lower speeds.

After making these choices, we roughly determined the amount of torque needed to turn each screw by using a torque wrench (Table 2). We only measured the monochrometer and side screw torques. These two measurements bounded the problem because the side screw clearly required the most torque and the monochrometer screw was much easier to turn than the other three.

With these measurements in mind, we chose motors that could easily handle the load. The ones that we selected are oversized by more than 110 percent (Table 3).
### Table 2—Torque Measurements

<table>
<thead>
<tr>
<th>Screw</th>
<th>Turning clockwise, lb-in.</th>
<th>Turning counterclockwise, lb-in.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Side</td>
<td>5.8</td>
<td>6.8</td>
</tr>
<tr>
<td>Monochrometer</td>
<td>3.0</td>
<td>2.4</td>
</tr>
</tbody>
</table>

### Table 3—Gear Motor Specifications

<table>
<thead>
<tr>
<th>Motor</th>
<th>Rated speed, rpm</th>
<th>Rated torque, lb-in.</th>
<th>Rated current, A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monochrometer</td>
<td>24</td>
<td>6.5</td>
<td>0.097</td>
</tr>
<tr>
<td>Other three</td>
<td>28</td>
<td>17.4</td>
<td>5.0</td>
</tr>
</tbody>
</table>

**Motor Mounts and Couplers**

To attach our motors to the tube housing, we created custom mounts out of aluminum. We chose aluminum because it is lightweight and is much easier to machine than other materials. Each mount was attached to the tube housing using already available features, with the exception of tapping several existing holes. We decided to attach the motors loosely to their mounts so that the motors would be free to move. This reduced the radial forces from any slight misalignment that could otherwise damage the motor’s bearings.

We also fabricated couplers to connect the motor shaft with the Allen wrench heads needed to turn the screws. The couplers were made from aluminum and attached using set screws. Figure 2 shows the motors mounted on the diffractometer.

**Motor Controller**

We selected a simple bidirectional H-bridge motor controller (Fig. 3) because it properly balanced control precision, simplicity, reliability, and build time for this project. The H-bridge type controller is capable of fairly precise speed control in either the clockwise or counterclockwise direction. It is capable of throttling from 0 to 100 percent. However, this throttling does not produce 0 to 100 percent speed control of the motor due to the numerous non-ideal factors of a DC motor’s response. Namely, winding losses, magnetic core hysteresis, the difference between static and dynamic friction, and other factors limit the actual control of the motor’s speed to approximately 10 to 100 percent. Those numbers were estimated during testing of the actual motor controller, motors, and tube housing.

Still, we decided that this level of control should be sufficient considering the gear motors’ full speeds of about 30 rpm. This means that the user can throttle the motors down to 3 rpm, or one revolution every 20 sec. If the user then precisely stops the motor with 0.2 sec precision, the position can be controlled to within 3.6°. Our testing showed that a human is capable of consistently recognizing a trigger condition and pressing a button or flipping a switch within 0.1 sec of that trigger. So we believe that 0.2 sec precision is reasonable for most users.

Additionally, the particular motor controller chosen used a very simple control scheme based upon four operational amplifiers. This solution is purely analog, making it easier to troubleshoot in the event that a component should malfunction. However, this chance should be very low due to the relatively minimal number of components used in the controller. We chose to purchase a fully assembled motor controller because we did not have time to design, select components, construct, test, and revise a new controller design from scratch.
Figure 2.—Motors mounted on diffractometer.

Figure 3.—Bidirectional H-bridge motor controller.
Main Electronics Box

The main electronics box houses the power supply, relays, motor controller, and other small electronics (Fig. 4). It is designed to sit inside the x-ray diffractometer’s cabinet. The box itself is made of thick ABS plastic and is oversized for possible future expansion.

Fuse

Power enters the box through the 120 V AC receptacle. The line wire was then immediately run through a 2 A fast-blow fuse. This fuse protects the system from excessive currents.

Power Supply

The power supply that we selected is a commercial quality unit rated for very long life (Fig. 5). It provides 5, 12, and –12 V. Additionally, the supply requires a minimum load, as shown in Table 4, which we supplied via three power resistors, one attached to each of the voltage outputs. We actually chose to supply half the manufacturer’s recommended minimum load, as our testing showed this condition was sufficiently stable for our system.

Power Resistors

As stated previously, three power resistors were added to supply a minimum load to the power supply (Fig. 6). They are attached to a piece of aluminum, which is located near the exhaust holes and serves as a simple heat sink for cooling.

![Figure 4.—Main electronics box.](image1)

![Figure 5.—The power supply in the main electronics box.](image2)

<table>
<thead>
<tr>
<th>Supply voltage, V</th>
<th>Recommended minimum load</th>
<th>Chosen load</th>
<th>Resistor value, ohms</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>2.0 A</td>
<td>1.0 A</td>
<td>5</td>
</tr>
<tr>
<td>12</td>
<td>500 mA</td>
<td>240 mA</td>
<td>50</td>
</tr>
<tr>
<td>–12</td>
<td>100 mA</td>
<td>60 mA</td>
<td>200</td>
</tr>
</tbody>
</table>
Relays

The main electronics box contains 5 relays (Fig. 7). Four of them connect the motor controller’s output to one of the four motors, depending on the position of the 5 position switch on the hand-held controller. The other relay connects 12 V power to the motor controller when the power switch is flipped on the hand-held and the push-button is pressed. These relays are all standard automotive 30 A relays. They were selected both for durability and for ease of replacement. They are also greatly oversized considering that the maximum expected load to one of the large motors is 5 A.

All relays have flyback diodes connected between the relay coil contacts. These diodes prevent a large voltage build up and spark when the relay is turned off due to the stored magnetic field in the coil. This significantly increases the lifetime of the switches which control the relays by reducing sparking during an opening condition.

Cooling

When we added power resistors to our design to provide minimum load to the power supply, we determined that the main electronics box would need a small cooling fan to eliminate any chance of overheating. We added a 60 mm fan that pulls air into the case and blows it over the major electronics. The air then exits through the back, flowing over the power resistors and carrying their heat out of the enclosure.

Serial and Motor Cables

The control cable connecting the main electronics box to the handheld controls is a 14-conductor, shielded, twisted-pair cable with a male serial connector on the end that connects to the main electronics box. The shielding consists of both foil and 90 percent coverage braid. It uses 28 gauge conductors which can handle 226 mA.

The motors are connected to the main electronics box through four custom cables. One end of each cable terminates in a two-position Molex connector, which mates with connectors on the main electronics box. The other end has quick connection terminals which slide onto the motor leads. The polarity of the connection with the motor leads is not critical, as flipping the connection will simply reverse the direction of rotation. We designed the system such that rotating the control knob on the hand-held clockwise will cause the selected motor to rotate clockwise, and vice versa.
Handheld Controller

The layout for our handheld controller is fairly simple (Fig. 8). We used a terminal block to allow easy access to certain voltage supplies and connections. We have an on/off switch, which controls power to the motor controller. When the switch is turned on, the red LED lights up. We also have a motor selection switch. The switch can be in one of the following five positions: None, M1, M2, M3, and M4. Positions M1 through M4 each operate a single motor. In the “None” position, no motor will be activated. A potentiometer controls the speed and direction of the motors. The farther the potentiometer is turned, the faster the selected motor will spin. However, the motor will only turn if the user presses the pushbutton. The pushbutton can be held in for large movements or pressed and released quickly for fine tuning.

Results

The alignment time goal was met. Motor installation, beam alignment, and motor removal were accomplished in less than half an hour. The design, commercial component procurement, mount fabrication, assembly, and testing were all performed by the authors within the span of the 10-week internship plus a 1-week extension for one of the authors to implement and test the momentary pushbutton feature of the handheld controller. The total cost of items procured for the project was under $900.
Appendix—Circuit Schematic
14. ABSTRACT
X-ray diffraction (XRD) is a powerful analysis method that allows researchers to noninvasively probe the crystalline structure of a material. This includes the ability to determine the crystalline phases present, quantify surface residual stresses, and measure the distribution of crystallographic orientations. The Structures and Materials Division at the NASA Glenn Research Center (GRC) heavily uses the on-site XRD lab to characterize advanced metal alloys, ceramics, and polymers. One of the x-ray diffractometers in the XRD lab (Bruker D8 Discover) uses three different x-ray tubes (Cu, Cr, and Mn) for optimal performance over numerous material types and various experimental techniques. This requires that the tubes be switched out and aligned between experiments. This alignment maximizes the x-ray tube’s output through an iterative process involving four set screws. However, the output of the x-ray tube cannot be monitored during the adjustment process due to standard radiation safety engineering controls that prevent exposure to the x-ray beam when the diffractometer doors are open. Therefore, the adjustment process is a very tedious series of blind adjustments, each followed by measurement of the output beam using a PIN diode after the enclosure doors are shut. This process can take up to 4 hr to perform. This technical memorandum documents an in-house project to motorize this alignment process. Unlike a human, motors are not harmed by x-ray radiation of the energy range used in this instrument. Therefore, using motors to adjust the set screws will allow the researcher to monitor the x-ray tube’s output while making interactive adjustments from outside the diffractometer. The motorized alignment system consists of four motors, a motor controller, and a hand-held user interface module. Our goal was to reduce the alignment time to less than 30 min. The time available was the 10-week span of the Lewis’ Educational and Research Collaborative Internship Project (LERCIP) summer internship program and the budget goal was $1200. In this report, we will describe our motorization design and discuss the results of its implementation.

15. SUBJECT TERMS
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