

Making the Laue More Accurate and User-Friendly

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Primary JHU PARADIM Tool Used: Laue diffractometer

Abstract

The Laue diffractometer is a useful tool to find the orientation of crystal samples. However, crystal alignment can be an arduous process due to the imprecise alignment tools that accompany the Laue, which require the user to “eyeball” whether a sample is properly aligned based on resulting diffraction patterns. In order to improve the usage of the Laue, a program was created that will eliminate the need for a joystick and allow the user to control the jack and translation stage, as well as the goniometer, from the computer. This is a crucial first step in automating the Laue and making it easier to use, especially in the age of Covid-19. With this program, it will be possible to work with the Laue outside of the lab and new possibilities are opened for Laue control and accuracy. Furthermore, with the motor parts fully interfaced with the computer it will be possible to create a program that allows the user to see the crystal diffraction pattern in real time and lets the user know how far in any direction the sample needs to move to reach a specific alignment in the crystal.

Introduction

The Laue diffractometer is a machine used to find the alignment of a crystal. It uses x-rays that reflect off of the atoms in a crystal sample and then onto a film, creating a diffraction pattern. Within each crystal there are unit cells that are the

simplest repeating structural unit. There are seven different primitive unit cell structures, that are arranged so that each unit cell shares an atom with another at the corners. These are the atoms that the x-ray reflects off of when analyzed with the Laue. Furthermore, different sets of planes fill the unit cell.

These planes are important because the properties of the crystal may change depending on what plane the crystal is oriented on. These anisotropic properties of certain crystals are why the Laue is so important. When the properties of a crystal sample are direction dependent the Laue is necessary to orient the crystal before performing tests on it. Without knowing the crystal's orientation, the other test results may be misleading.

The Johns Hopkins lab currently has an MWL 110 Laue as pictured in Figure 1. This model includes motorized parts that help position the crystal, in addition to the diffraction parts. These motorized parts are controlled by a joystick that sends signals to the motor driver which then tells the motor parts to move. Using the joystick, the user can orient their crystal however they want. However, the Laue has no way of showing the user where the crystal is oriented until the diffraction pattern is taken. This means that the user has to constantly adjust the crystal position and re-take the diffraction pattern until they get an image that is more or less on the mark.

In order to fix this issue, the joystick must be replaced with a user-friendly computer program. This program will control the motorized parts in the Laue and provide data to the user in real time. This includes: how far to go in a given direction to reach a given plane as well as where the crystal is currently oriented. By eliminating the joystick, this program will also reduce maintenance and make the Laue accessible remotely.

Summary of research:

Interfacing the moving parts of the Laue with the computer required LabView, a graphical software program, to write the code. The first task was to create a simulation mimicking how the program would work with the motorized parts of the

machine. This simulation consisted of a 3D cube and a panel of buttons. Each button on the panel moves the cube in the indicated direction. As the cube moves there is a position readout that tells the user how far in any direction the cube has gone from the origin. Additionally, the user is able to move the cube in varying step sizes. The actual motorized parts of the Laue move in specific step sizes, so in order to implement this step size choice, the user chooses how many steps the cube should take in a single push of the button rather than actually changing the size of each step. The simulation buttons are also divided according to motor pairs as pictured in Figure 2, which refers to the motorized part being controlled in the actual machine.

In order to transfer the program from simulation to real life a set of relays is required to physically replace the joystick. The code communicates with a certain relay that switches on the relevant motor pair. After that another signal will tell a relay that correlates to a certain direction to switch on. Each direction is associated with a specific voltage that is sent to the motor driver. These relays will be connected to the computer via USB port.

Future Goals:

Once the Laue is fully interfaced with the computer it will be possible to create a program that presents the diffraction pattern tracks the orientation of the crystal in real time. This program will also tell the user how far they are from a certain plane and recommend how many steps to take in any direction to get there. This is extremely important in order to take away the guesswork in orienting the crystal sample and will make the Laue significantly easier to use.

Conclusion:

As it stands, using the Laue involves a lot of guesswork, maintenance and time. However, the programs described above will remedy these issues and open doors for further improvement. For example, the program can be fitted with a real-life camera view of the sample so that the user has a better idea of where the sample is in relation to the rest of the machine. This is especially useful for users who are outside of the lab and would like that extra visual. Another possibility is allowing access to the computer program through a smartphone or tablet so if someone in the lab wants to adjust the position of the crystal from different spots on in the lab, they can. The Laue is an incredibly important tool in the research of crystals and should be as accurate and user-friendly as possible.

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References

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Figures:



Figure 1. MWL 110 Laue in Johns Hopkins. A. Laue, A.i. 3-axis goniometer, A.ii. jack and translation stage, B. joystick, C. Motor Driver.

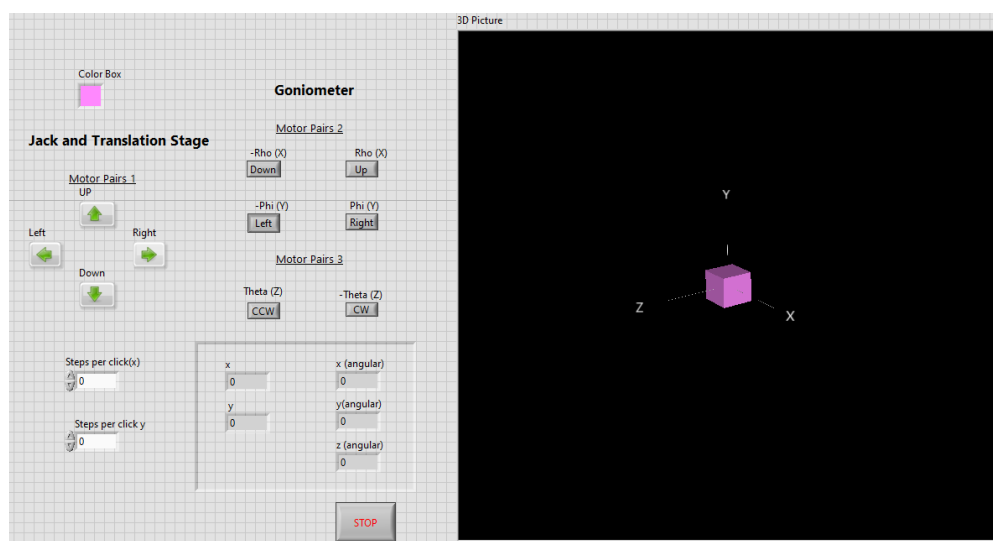


Figure 2. Front panel of simulation. Motor pair one refers to the jack and translation stage that moves the sample in the x and y direction. Motor pair two, controls the movement of the goniometer in the x and y direction and is shown as the rotation around the respective axes in the simulation. The third motor pair controls the rotation of the barrel at the top of the goniometer

and is represented as the rotation around the z-axis.