

Using a PC-based LabVIEW Program for Acquiring and Processing X-Ray Diffraction Data

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The Challenge: Upgrading X-ray powder diffraction (XRPD) systems used for analyzing minerals, rocks, ceramics, soil, and metals in industry and academia.

The Solution: Using National Instruments LabVIEW and a PCI data acquisition board to collect, process, and present X-ray diffraction for both qualitative and quantitative analysis.

Introduction

XRPD is a powerful method for the qualitative identification of crystalline materials and their quantitative analyses. The new generation of X-ray diffractometers now interfaces with an expensive proprietary computer system. Yet many X-ray diffractometers are without such automation, and it is rather costly to upgrade them. The automation with LabVIEW is much simpler and less expensive at one-third of the current cost. With National Instruments plug-in PCI-MIO-1 6XE-50 data acquisition board, we can connect the intensity data from the existing X-ray diffraction system to a PC. As a result, we have developed software to collect, process, and present X-ray diffraction data for both qualitative and quantitative analyses.

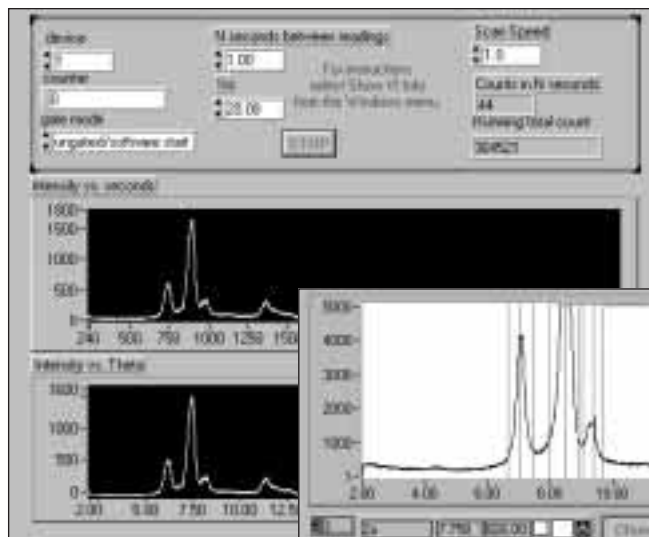
Program Design

The software consists of two parts:

- Data acquisition program called “Acquire XRD”
- Data processing program called “Process QXRD”

Data Acquisition Acquire XRD

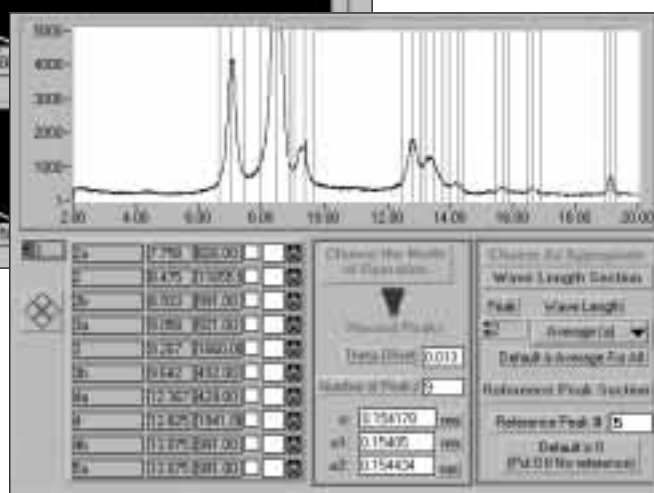
The LabVIEW program collects the digital signal from the X-ray detection system as an (x, y) matrix, with x being the selected time interval at a given scanning speed of the X-ray diffractometer, and y being the number of counts (intensity) received by the X-ray nuclear counter. The data is then saved as a data file, so the “Process QXRD” program can process it offline.



Left: Screen showing acquired XRD raw data

Data Processing

This program first presents the saved data as a time/intensity plot and then converts it into an intensity/diffraction angle (two-theta) graph, considering the variables of the experiment such as scanning speed of the X-ray diffractometer and the time interval for collecting the digital signal. The user precisely marks the peak positions of the individual X-ray reflections with the cursor. The initial and final locations of the background points define the reflection. We do not use a statistical calculation of the selections of these positions because it often generates erroneous results while



Below: Screen showing processed XRD data

differentiating low intensity peaks from the background. Though the manual selection of the peak and background positions with cursors is a time-consuming process, it is far more precise than using statistical calculations.

The program allows the options for calculating the integral intensity or peak intensity with background corrections in each case. It calculates absolute and normalized intensities for all or selected reflections.

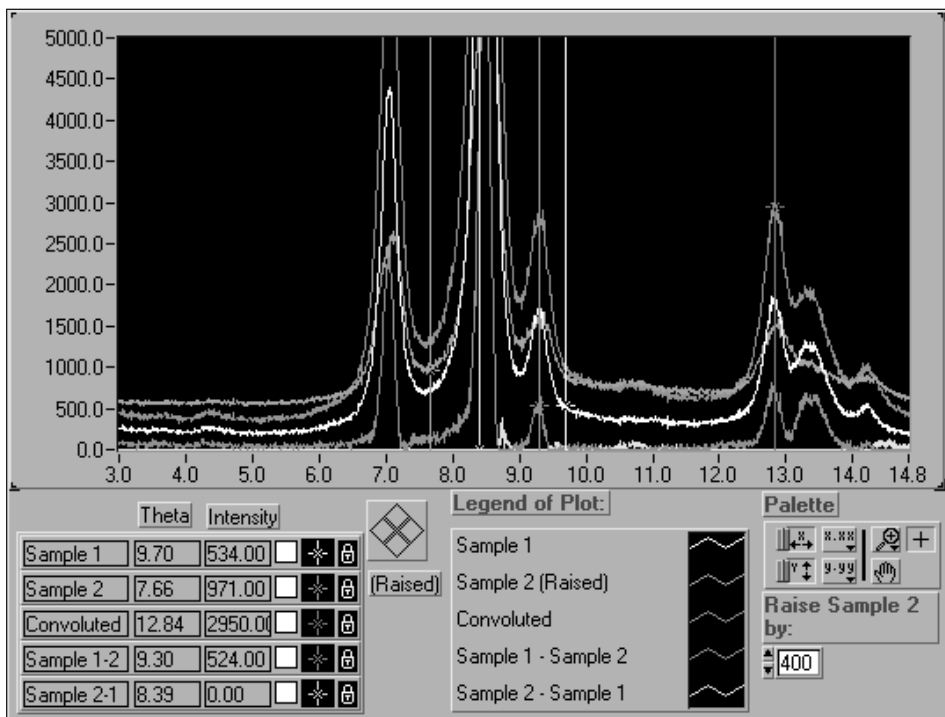
We can select one of the reflections as a reference line, and as a result, the program will calculate reference intensity ratios for quantitative X-ray diffraction analysis.

Data Presentation

An Excel file in the form of a table presents the d-spacings and intensities corrected for

n	Theta	Integrated Intensity	Relative Intensity	d in nm
1	4.41	3390	1	1.003
2	7.07	149595	34	0.627
3	8.48	446102	100	0.523
4	9.29	31383	7	0.477
5	12.83	36446	8	0.347
6	13.28	27455	6	0.336
7	14.20	5441	1	0.314
8	15.23	1924	0	0.293
9	15.63	4527	1	0.286

Data Presentation



Screen showing processed XRD data

background. The X-ray diffraction pattern displays along with the tabulated data and the program marks all the analyzed reflections with sequential numbering. Now, we can plot several patterns on the same graph and add or subtract two patterns point-by-point from each other. We can also use this for convolution or deconvolution of X-ray reflections.

System Detail

Data acquisition and data analysis are the center of this system, both of which we achieved with the use of LabVIEW. For data acquisition, we used the DAQ board along with the SCB-68 accessory. These aid in collecting digital pulse counts directly from the nuclear counter of the X-ray

diffractometer in a very efficient manner. The system block diagram shows the signal flow direction at data acquisition time.

The program, Acquire XRD, drives the devices mentioned above in collecting the data. Because of its ease of use and in manipulation of graphs and charts, the plots for previously acquired X-ray data are simple and easy to read. We can readily obtain several options such as reference peak, wavelength for individual reflections, automatic theta correction (offset), peak and background intensities on the screen.

Reduced Costs

LabVIEW and the NI data acquisition board provide a practical and economic option for the acquisition and processing of X-ray

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diffraction data, which could significantly reduce the cost of automation for the manufacturers of future X-ray diffraction systems. Moreover, as we have demonstrated in our laboratory, it is easy to update existing systems without automation and at a reasonable cost using these NI products. ■

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