

WinXRD: Data Collection and Analysis Package

ARL X'TRA XRD SYSTEM

Product
Description

Nr. XRD-5

Introduction

WinXRD is a true multitasking 32-bit data collection and analysis package that runs under Microsoft Windows NT and 2000®. This comprehensive software package is fully integrated and facilitates a smooth progression from data collection through analysis and report writing.

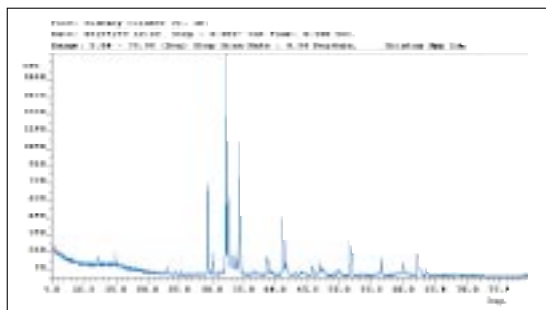
The analytical algorithms include:

- Background removal and smoothing;
- Peak finding and profile fitting;
- Data file manipulation for scaling, adding and subtracting;
- Qualitative and quantitative analysis;
- Percent crystallinity determination;
- Crystallite size determination by Scherrer, Williamson-Hall and Warren-Averbach methods;
- Texture and residual stress analysis;
- Indexing and least squares unit cell determination.

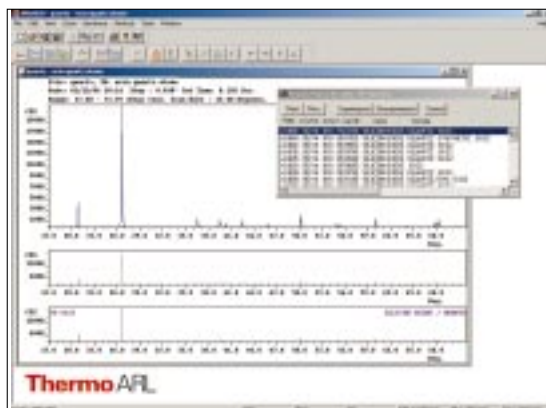
Full batch processing of multiple hardware and analysis applications allows printer and plotting operations.

An integrated control system handles all hardware adjustments through screen menus.

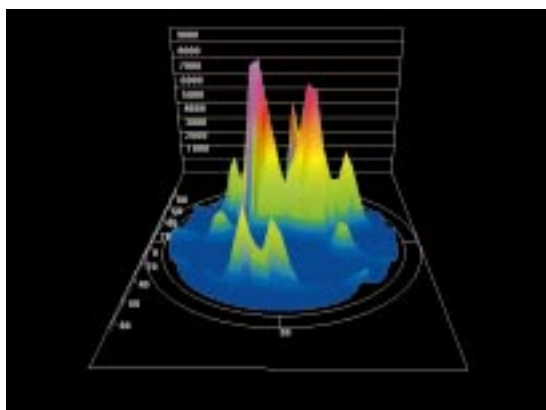
Applications



Raw scan of a cement clinker sample



Qualitative (Search/Match) analysis using ICDD data base



Pole figure of an aluminum foil in 3-D

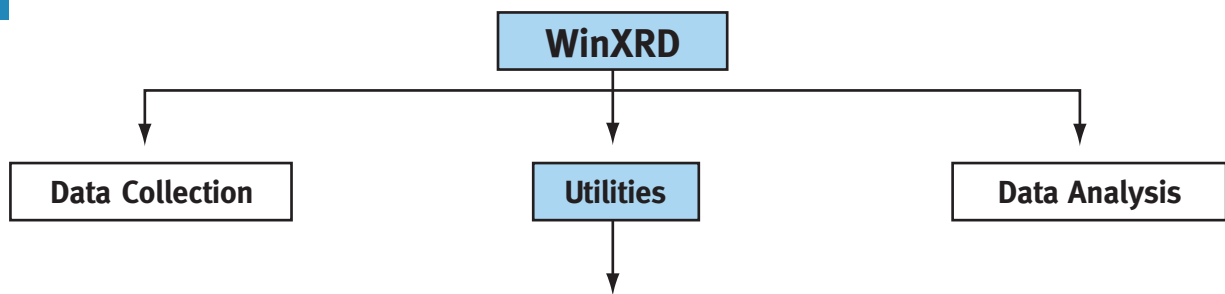
WinXRD

Data Collection

Utilities

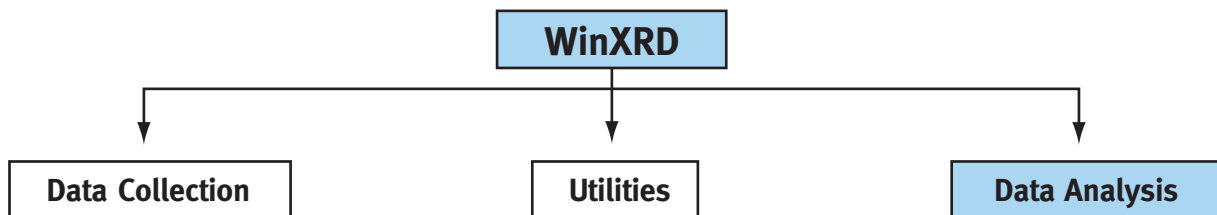
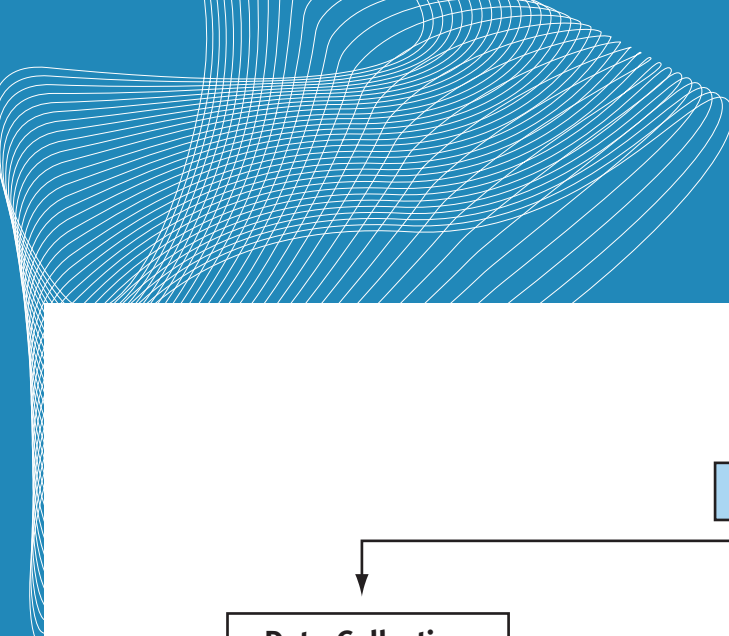
Data Analysis

Data Scan	<ul style="list-style-type: none"> • Normal Scan • 2-Theta Scan (Grazing Angle Scan) • Omega Scan (Rocking Scan) • Multi Axis Scan 	These are the standard scan routines. Three scans (normal, 2-Theta and Omega) are used on two-axis diffraction systems. 2-Theta scans are used to study thin films or surfaces in grazing angle geometry. Omega scans are used to study crystallite orientation. The single and multi-axis scans are used on systems with more than two axes.
Controlled Atmosphere Scan	<ul style="list-style-type: none"> • High Temperature Scan • High/Low Temperature Scan 	These data collection routines allow collection of diffraction data while simultaneously controlling the sample temperature and/or gas environment using a temperature stage and/or gas control system. These data can be displayed in 3D with our Multigraph program.
Instrumental Parameter Scan	<ul style="list-style-type: none"> • Standard Database Generator • Auto Scan Range Calculator • STD File Generator 	These data collection routines collect information on diffractometer alignment using a standard sample such as NIST SRM 1976 corundum plates. These data are used by the Instrumental Standard Analysis package.
Polefigure Scan	<ul style="list-style-type: none"> • Step and Continuous Scan • Grazing Angle Polefigure Scan • Auto Background Subtraction 	These scan routines collect diffraction data to study sample texture. These data are displayed with our Polefigure Analysis program.
Stress Scan	<ul style="list-style-type: none"> • Step and Continuous Scan • PSI Increment in Linear or \sin^2 PSI • Depth Profiling Scans • Biaxial 	These scan routines collect diffraction data used to measure the amount of residual stress in a solid sample. These data are used by our Residual Stress Analysis package.
Retained Austinite Scan	<ul style="list-style-type: none"> • Fuzzy Logic Step or Continuous Scan • Auto Profile Fitting Calculation • Auto Preferred Orientation Calculation • Auto Symmetry Calculation 	These routines collect data used to calculate the concentration of martensite and austinite in steel. These routines are based on SAE method SP-453 and feature automatic profile fitting and on-the-fly compensation for sample texture. These data are used by the Retained Austinite Analysis program.

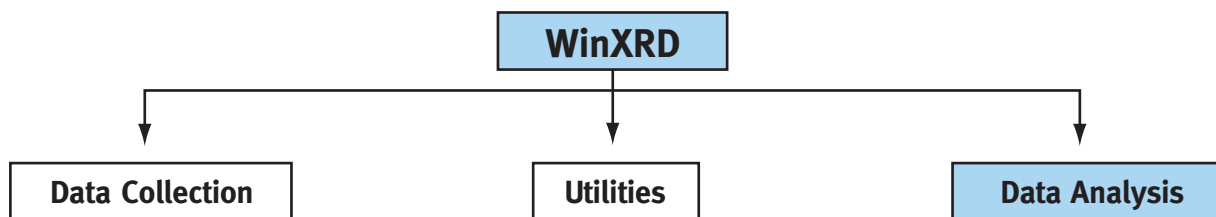


Data File Editor
Reference Information Database Creator (IDB)
Data File Export <ul style="list-style-type: none">• .raw• multiple .raw• .ni• .pk• .rd• .mrw• .epf• GSAS• Beartex• ASCII• Search Match
Data File Import (ASCII)*
Data File Wavelength Converter
Data File Superimpose
Data File Property Viewer
Artificial Data File Generator
Graphics Export to Bitmap and Metafile

* Create .raw files from other exported .raw files.

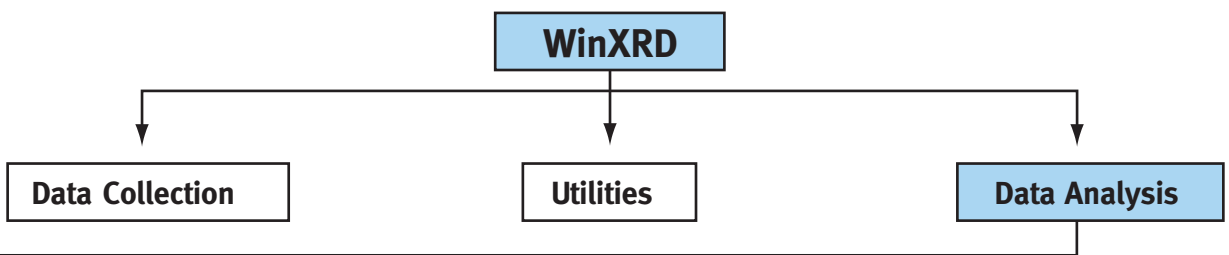


Data Reduction	<ul style="list-style-type: none"> • Background Correction <ul style="list-style-type: none"> - Auto/Manual Operation - $K\alpha_2$ Stripping • Noise Cancellation <ul style="list-style-type: none"> - Fast Fourier Transform - Boxcar Smoothing • Peakfinding <ul style="list-style-type: none"> - Digital Filtering Method - Profile Fitting Method • Profile Fitting Methods <ul style="list-style-type: none"> - Split/Sym. Pearson VII - Lorentzian - Gaussian • Peak Editor <ul style="list-style-type: none"> - Peak Insertion - Peak Deletion - Peak Parameter Editing - Lattice Parameter Edit 	<p>These programs are used to strip background and $K\alpha_2$ from the raw data. Several peakfinding routines will provide peak location and intensity. Manual insertion and deletion enhance data file integrity.</p>
Qualitative (Search/Match) Analysis	<ul style="list-style-type: none"> • PDF-1 and PDF-2 Standard and Fuzzy Logic Search • Periodic Table Filter • Search Logic Filter • ICDD Database Generator • User Database Generator • ICDD Card Search and Display 	<p>This program analyzes a diffraction pattern for the presence of phases based on the ICDD or user database. PDF-2 database uses a fuzzy logic search algorithm. A periodic table and chemistry logic can be applied to restrict the search.</p>
Pattern Simulation/ Manipulation	<ul style="list-style-type: none"> • Generate Diffraction Patterns from ICDD or Personal Files • Generate New Pattern from Multiple Phases • Set Desired Peak Parameters • Linear or Non-Linear Background Generation with Random Counts • Add, Subtract and Scale Two Patterns 	<p>This program has two modes; data file creation and data file manipulation. A data file can be created by ICDD input or by specifying peak information. Also, a data file can be created by adding, subtracting or scaling two existing data files.</p>

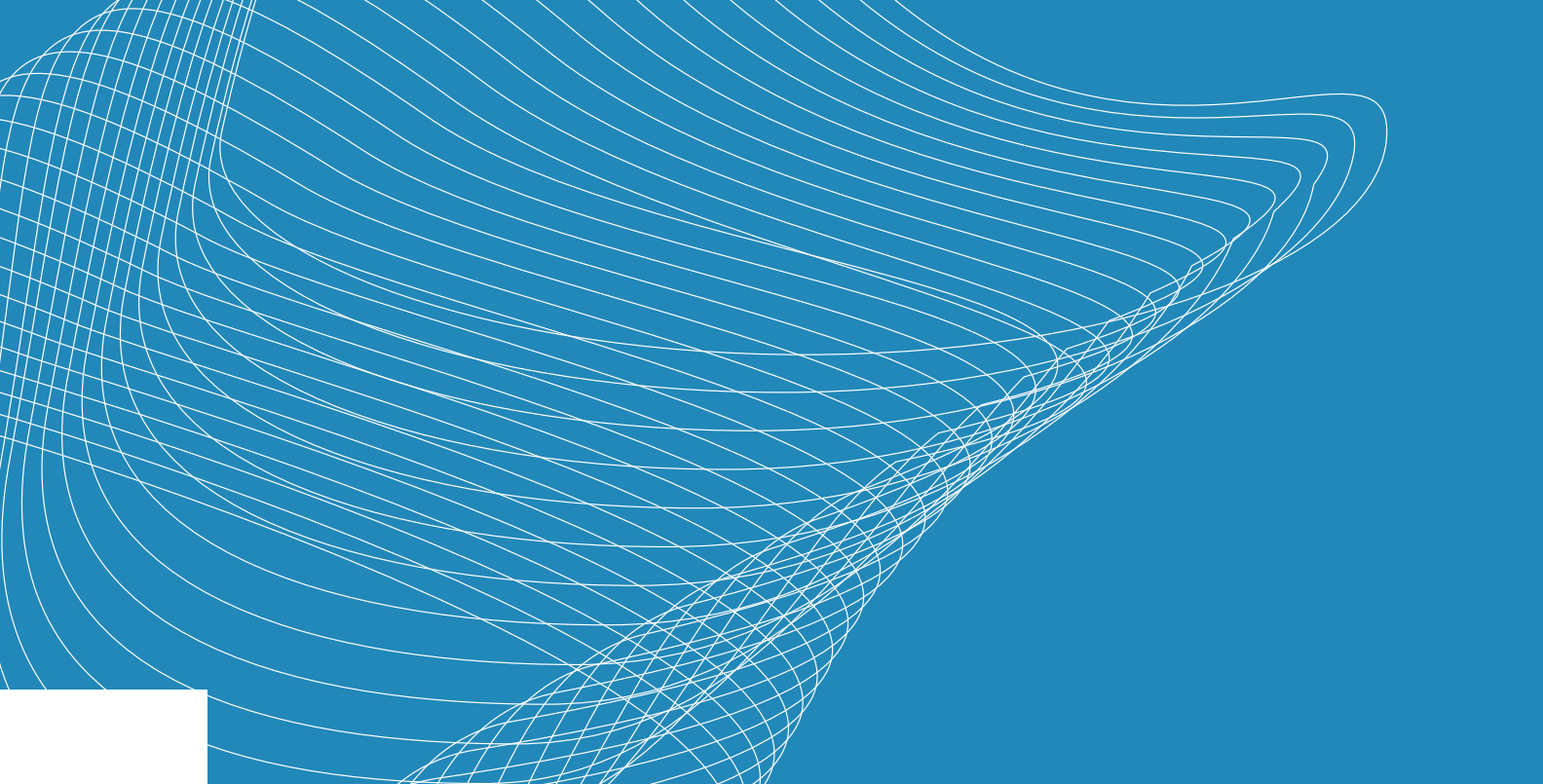


Multi-Graph Display	<ul style="list-style-type: none"> • 3D Display with Multiple Data Files • Zoom, Rotate 3D Display • Determine Peak Position and Area in 3D Model • View 3D Model Axes • On-Line Help 	<p>This program allows the visual representation in 3D of a series of related data files. This is most useful for a series of files collected at different temperatures.</p>
Polefigure Analysis*	<ul style="list-style-type: none"> • 3D Display of Polefigure Data • Zoom, Rotate 3D Display • View 3D Model Axes • 2D Display of Polefigure Data • Stereographic and Equal Area Projections 	<p>These programs display the results of a sample texture measurement for a particular diffraction plane in 2D or 3D. Combining the results of two or more polefigures allows the determination of orientation distribution functions (ODF) using the 3rd party PopLA or Beartex programs.</p>
Residual Stress Analysis*	<ul style="list-style-type: none"> • Biaxial, Triaxial and Triaxial with Shear Calculations • Materials Database Generator • Gradient Correction Calculation • S₁ and 0.5S₂ Calculations from Single Crystal Information • Subsurface Stress Calculations 	<p>This program determines the 3D residual stress tensor in solid samples from small changes in lattice parameters. The program can also determine and correct for the presence of subsurface stress gradients.</p>
Quantitative Analysis	<ul style="list-style-type: none"> • External Standard Method (different from matrix) • Internal Standard Method (same as matrix) • RIR Method • Standard Addition Method 	<p>This program provides four methods for determining the concentration of one or more phases in a mixture of phases.</p>
Crystallography	<ul style="list-style-type: none"> • Manual Indexing • Automatic Indexing Treor • Lattice Refinement • Peak File Editor 	<p>These programs aid in the calculation of lattice parameters and Miller indices for polycrystalline materials. Treor attempts to automatically calculate crystal system, lattice parameter and Miller indices based only on a peakfile. Lattice refinement calculates lattice parameters based on an initial guess or on an assigned Miller index. It is also possible to manually assign miller indices using the programs.</p>

* See 3rd party software page



% Crystallinity Analysis	<ul style="list-style-type: none"> • Calculate Percentage of Crystalline versus Amorphous Material • Amorphous Area Editor • Peak Area Editor • Region of Interest Generator 	This program estimates the percentage of crystalline material in a mixture of amorphous and crystalline materials.
Crystallite Size Analysis	<ul style="list-style-type: none"> • Scherrer Method • Warren-Averbach Method • Williamson/Hall Method • Step-by-Step Program Tutorial 	This program determines crystallite size by examining peak broadening in a polycrystalline diffraction sample.
Retained Austenite Analysis	<ul style="list-style-type: none"> • Automatic Background Correction • Automatic Profile Fitting Calculation • Auto Preferred Orientation Calculation • Auto Symmetry Calculation 	This program determines the ratio between austenite and martensite concentration in steel.
Instrumental (Internal/External) Standard Analysis	<ul style="list-style-type: none"> • Automatic Background Correction • Automatic Profile Fitting Calculation • Reference Information Database Creator • Visual Representation of Instrument Conditions 	This program makes corrections to a peakfile based on an internal or external standard file. A graphics output is provided to display instrument conditions.



WinXRD



Third Party Software Solutions



Sietronics	<ul style="list-style-type: none">• MINDI: Mineral Structures Analysis• SIROQUANT: Quantitative Analysis	Available at: http://www.sietronics.com.au/siroqnt/siroqnt.htm
GSAS	<ul style="list-style-type: none">• General Structure System	Available for download from: ftp://ftp.lanl.gov/public/gsas/ Robert Von Dreele E-mail: vondreele@lanl.gov
Beartex	<ul style="list-style-type: none">• Polefigure Analysis	Available through Rudi Wenk at UC Berkeley: beartex@seismo.berkeley.edu http://www.seismo.berkeley.edu/~wenk/beartex.htm
popLA	<ul style="list-style-type: none">• Polefigure Analysis	Available for download from: http://www.lanl.gov/orgs/mst/cms/poplalapp.html John Bingert E-mail: bingert@lanl.gov

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Other offices, representatives and service centres
are located throughout the world



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