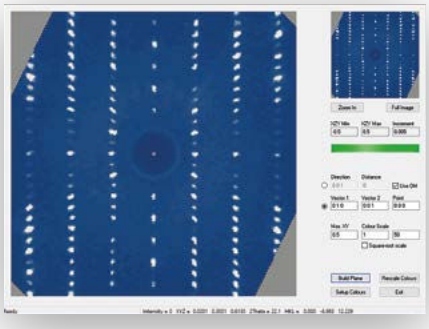
STOE

SINCE 1887

X AREA
SINGLE CRYSTAL DIFFRACTION SOFTWARE

THE STOE SINGLE CRYSTAL DIFFRACTION SOFTWARE PACKAGE



SINGLE CRYSTAL DIFFRACTOMETRY

X-Area is the complete, easy to use, yet flexible and powerful software package for data collection and evaluation on the **STOE STADIVARI** and **STOE IPDS** diffractometer series

- Highest quality of unit cell and intensity data
- SHELX-compatible intensity data sets and direct connection to Olex2
- Liberal license policy: lifetime free software updates and license for unlimited use in your department

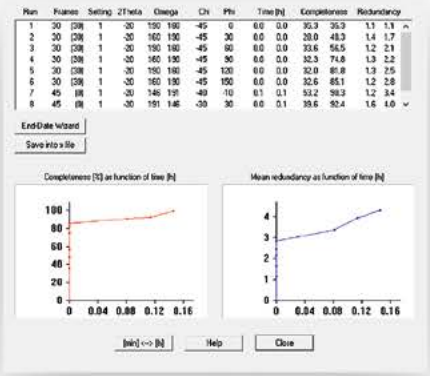
YOUR PARTNER IN X-RAY DIFFRACTION

STOE & Cie GmbH | WWW.STOE.COM

DATA ACQUISITION

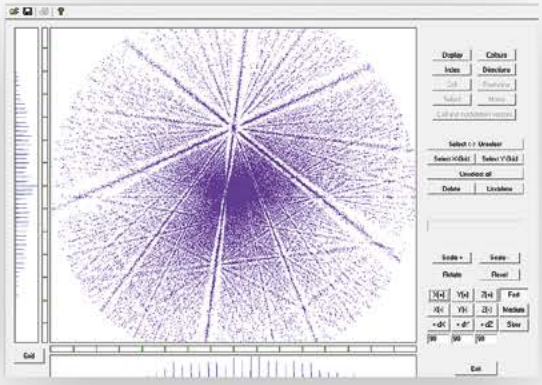
INSTRUMENT CONTROL / MEASUREMENT / RUN OPTIMIZER

- Intuitive interface to the diffractometer
- Easy centering of the sample with Faceit[Video]
- Automated data collection started with just a few clicks
- Run Optimizer calculates best measurement strategy according to user's requirements: completeness, speed & end time (with EndDate wizard)



RUN OPTIMIZER

Powerful Tool for enabling time-optimized data collection



ROBUST INDEXING

Graphics supported indexing enables full control of the crystal quality

DATA PROCESSING

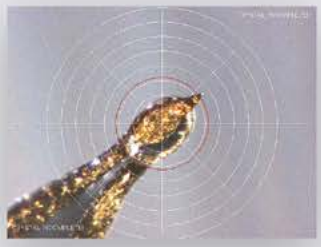
INDEX / CELL / REFINE

- Peak-finding routine scans frames rapidly in multi-processing mode
- Resulting peaks can be indexed either automatically or based on a robust graphical method
- Unit-cell parameters are refined according to the crystal system
- Unlimited number of peaks for the refinement

PRESENTATION

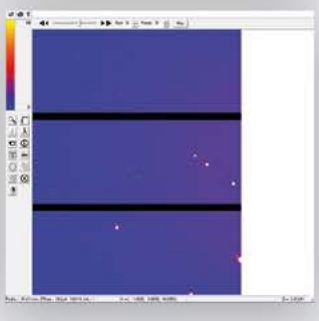
FRAME GRAPHICS

- X-Area offers a comprehensive graphics program for the inspection of collected frames
- Diffraction patterns can be checked for anomalous effects, e.g., twinning diffuse scattering etc.
- Toolbox offering various analysis options
- User friendly tool to create 1D powder diffraction patterns from 2D data including multiple file im- and export and supporting dual beam setups



CRYSTAL MONITORING

Video-camera signal to enable user-friendly crystal centering or even face indexing, if needed



REFLECTION INSPECTION

Sophisticated graphics software for a direct and easy inspection of the frames

INTEGRATION

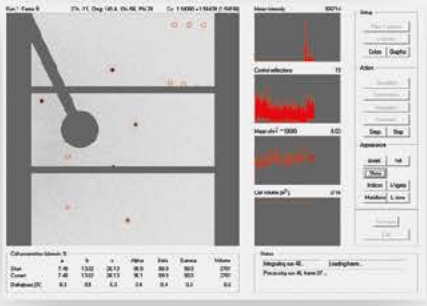
X AREA SINGLE CRYSTAL DIFFRACTION SOFTWARE

USE OF 3D INTEGRATION PROFILES

- Automatically adapting to the reflection profile for improved I/σ(I)
- Especially boosting weak data
- Automatic handling of α_1/α_2-splitting and overlap

USE OF EPILLEPTICAL REFLECTION PROFILES WITH

- Optional automated optimization of integration parameters
- α_1/α_2-splitting option for integration process
- Self-acting detection of reflection overlap
- Graphical control over the integration process
- Masking of user-specified detector areas possible



REFLECTION INTEGRATION

Reliable integration procedure provides accurate intensity data set

LAUE ANALYZER

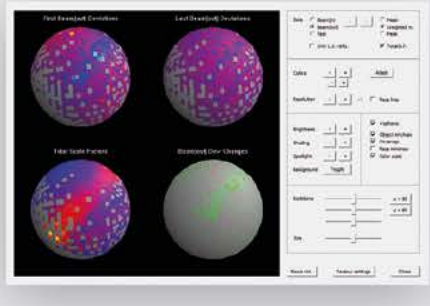
Quick and easy check of the Laue group including various diagnosis tools

DATA ANALYSIS

- E-statistics plot in order to control if space group is centrosymmetric
- Analyzer for convenient determination of the correct Laue group
- Automated space-group determination
- Display of peaks in reciprocal-space viewer
- Inspection of difficult patterns with layer representations in a reciprocal-space coordinate system, built from collected frames

DIAGNOSTICS

- Easily accessible overview of data quality through graphical representations of reflection groups
- Full statistical information on reflection groups and individual reflections within the chosen group
- R_{int} statistics over full measurement
- Individual reflections traceable on measurement frame
- Straight-forward outlier detection and simplified detection of their origin
- Easily accessible representation of scaling quality

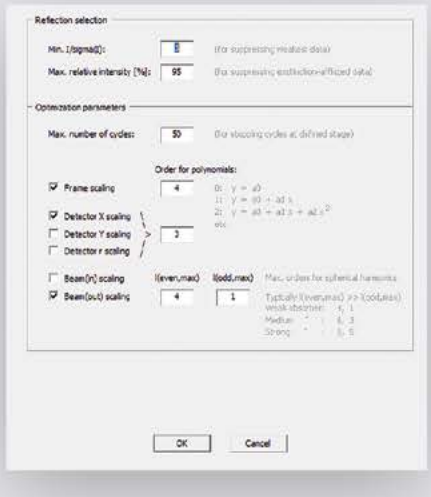


SPHERES

Visual tool to understand the quality of the applied scaling

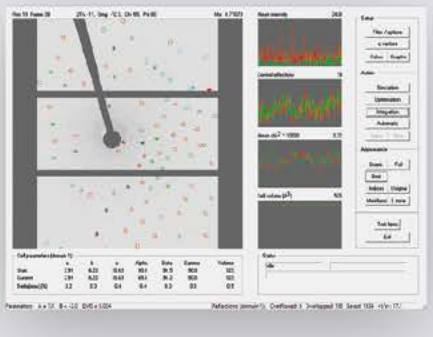
CORRECTIONS

- Lp and air-absorption correction
- Correction of absorption of X-rays by crystal (numerical correction or intensity scaling based on spherical harmonics in conjunction with symmetry-related reflections)
- Automated version of STOE's X-Shape
- Inter-frame scaling, based on polynomials
- Correction of crystal decomposition
- Rejection of outliers



SCALING

Scaling parameters can be individually set



MULTI-DOMAIN INTEGRATION

Example of a two-domain integration (turquoise: groups of overlapping reflections)

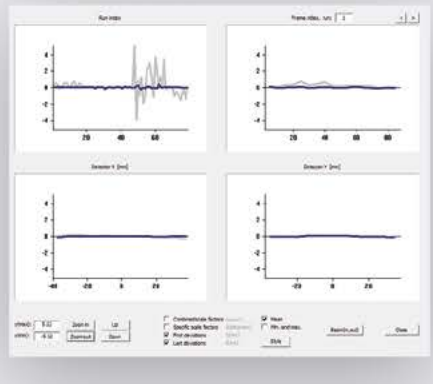
CHALLENGING STRUCTURES

MULTI-DOMAIN SYSTEMS

- Semi-automated indexing of peaks of the individual domains
- Simultaneous integration of intensities from up to eight individuals, full graphics control
- Intensity scaling based on sets of symmetry-related reflections

INCOMMENSURATELY MODULATED STRUCTURES

- Evaluation of the main lattice
- Determination and refinement of up to 3 q vectors
- Integration of main reflections as well as satellites
- Ability to process patterns from multi-domain crystals being incommensurately modulated
- Scaling of multi-domain, incommensurately modulated data according to operators choice, also including satellites



DIAGNOSTIC DIAGRAMS

After scaling intensity data, the improvement can be checked visually

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