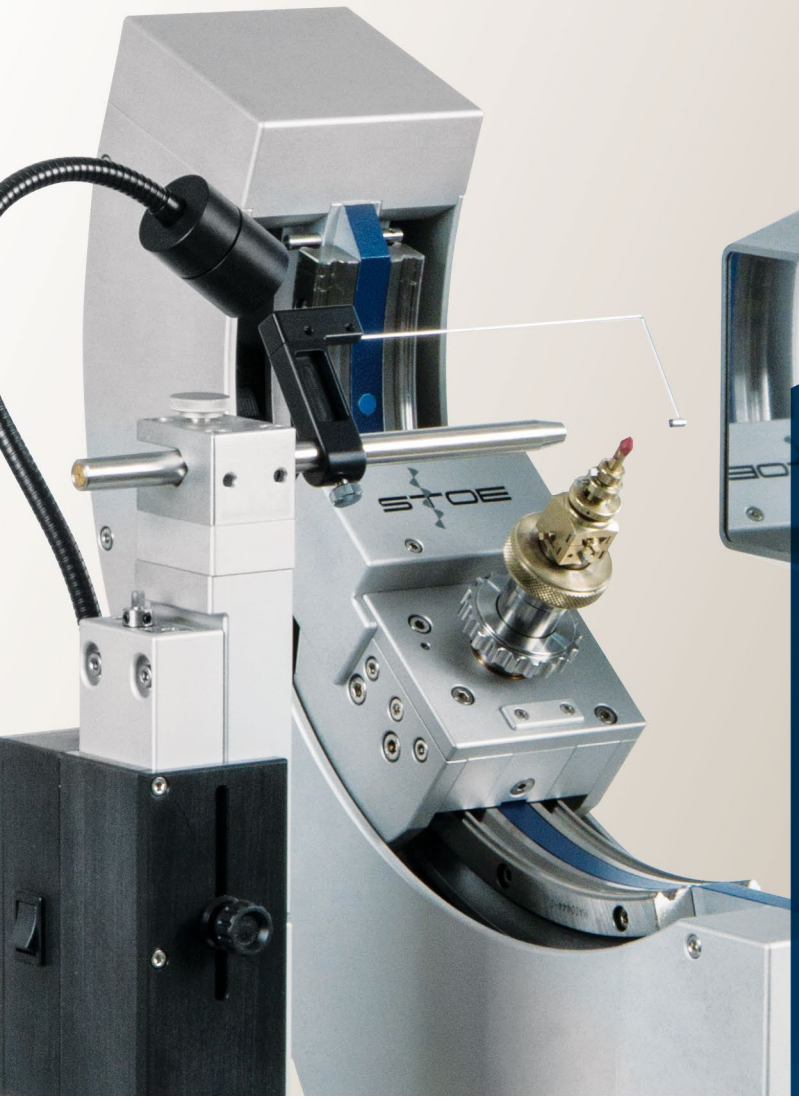
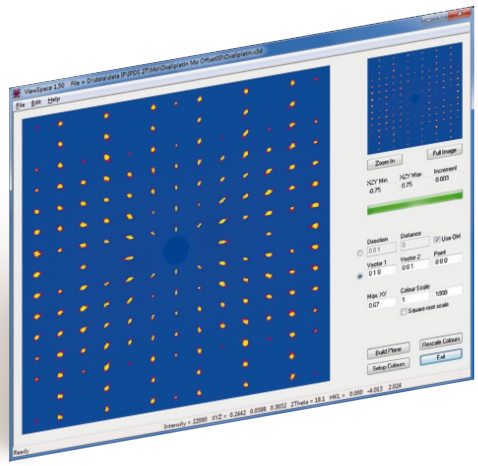
STOE

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 area detector software package for data collection and data evaluation on the STOE STADIVARI and STOE IPDS diffractometer series

- Highest quality of unit cell and intensity data
- Providing SHELX-compatible intensity data sets
- Full integration of STOE's Faceit^{Video} and X-Shape
- Liberal license policy: free software updates for 3 years, license for unlimited use in your department

YOUR PARTNER IN X-RAY DIFFRACTION

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SINGLE CRYSTAL DIFFRACTION

X AREA
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DATA ACQUISITION

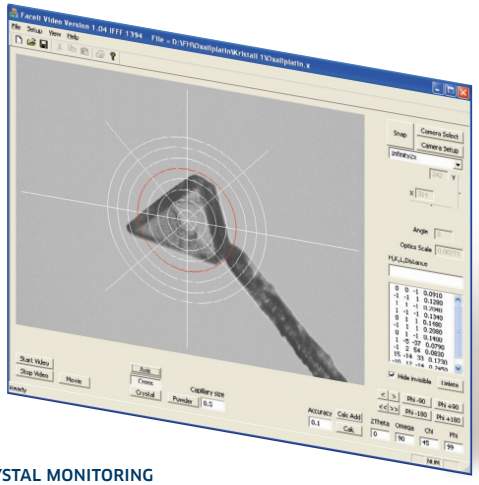
INSTRUMENT CONTROL / MEASUREMENT / RUN OPTIMIZER

- Intuitive interface to the diffractometer, offering direct access to all functions
- Easy centering of the sample with the aid of the integrated Faceit^{Video} function
- Automated data collection is started with just a few steps in the measuring program
- Frames with 32 bits per pixel facilitate high data accuracy
- User-friendly GUI optimizes the run strategy (e.g. in terms of high data completeness according to the crystal system and orientation), allowing faster and more dedicated collection of the data

PRESENTATION

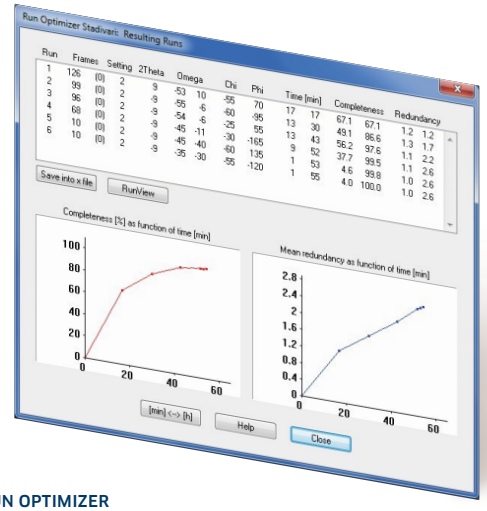
FRAME GRAPHICS

- X-Area offers a comprehensive graphics program for the inspection of collected frames
- Interactive display options provide an easy-to-use way for checking the quality of the crystal to be investigated, e.g. unexpected splitting of reflections can be examined easily
- Diffraction patterns can be checked for anomalous effects, as diffuse scattering



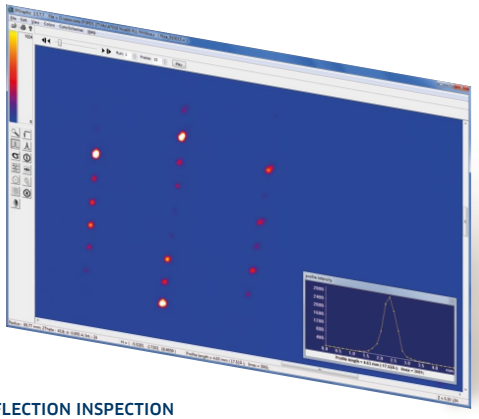
CRYSTAL MONITORING

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



RUN OPTIMIZER

Powerful tool for enabling time-optimized data collection



REFLECTION INSPECTION

Sophisticated graphics software for a closer look on the frames

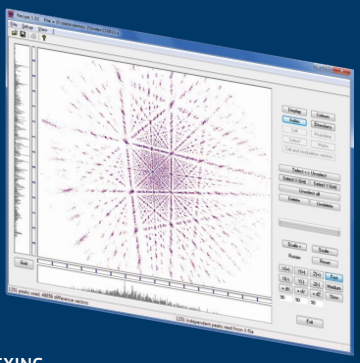
IMAGE PROCESSING

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 graphics method
- Unit-cell parameters are refined according to the crystal system
- Unlimited number of peaks for the refinement

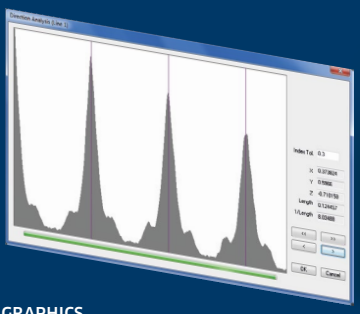
INTEGRATION

- Use of elliptical reflection profiles and α_1/α_2-splitting option for integration process
- Automated optimization of integration parameters
- Self-acting detection of reflection overlap
- Graphical control over the integration process
- Masking of user-specified detector areas possible
- Support of high-pressure cells by automatically calculated shading masks
- SHELX-compatible intensity data file by default
- XD-compatible file as an option



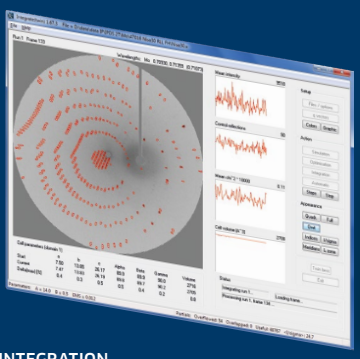
ROBUST INDEXING

Graphics supported indexing enables full control of the crystal quality



CONTROL BY GRAPHICS

During indexing, special effects as satellites may be detected easily

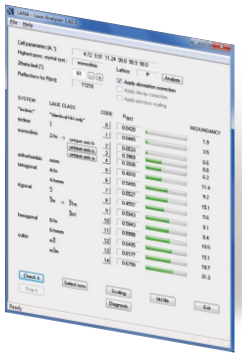


REFLECTION INTEGRATION

Reliable integration procedure provides accurate intensity data set

DATA ANALYSIS

- E-statistics plot in order to decide whether space group is centrosymmetric
- Analyzer for convenient determination of the correct Laue group
- Automated space-group determination
- Display of peaks in reciprocal-space viewer
- Difficult patterns can be inspected with the aid of layer representations in a reciprocal-space coordinate system, built from pixels of the collected frames
- Transformation of frame pixels into “powder diagrams”



LAUE ANALYZER

Quick and easy check of the Laue group

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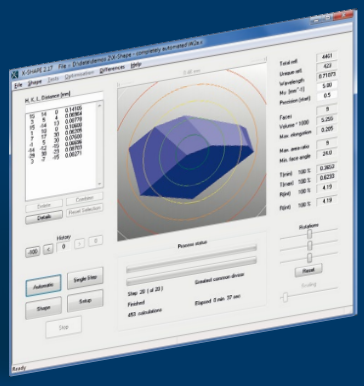


X-SHAPE
Automated crystal-shape optimization for numerical absorption correction

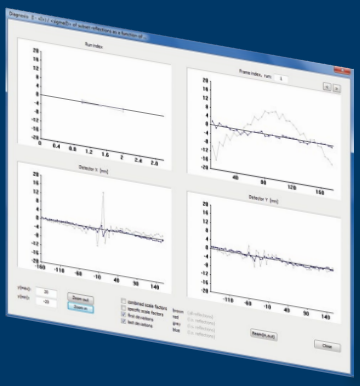
CORRECTIONS

- 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

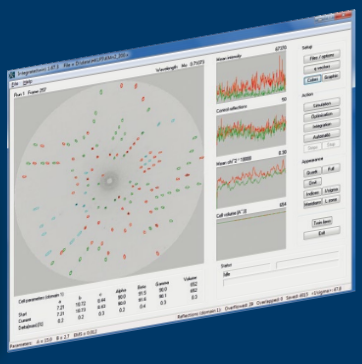
EXTENDED ISSUES

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



DIAGNOSTIC DIAGRAMS
After scaling intensity data, the improvement can be checked visually



MULTI-DOMAIN INTEGRATION
Example of a two-domain integration (turquois: groups of overlapping 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

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