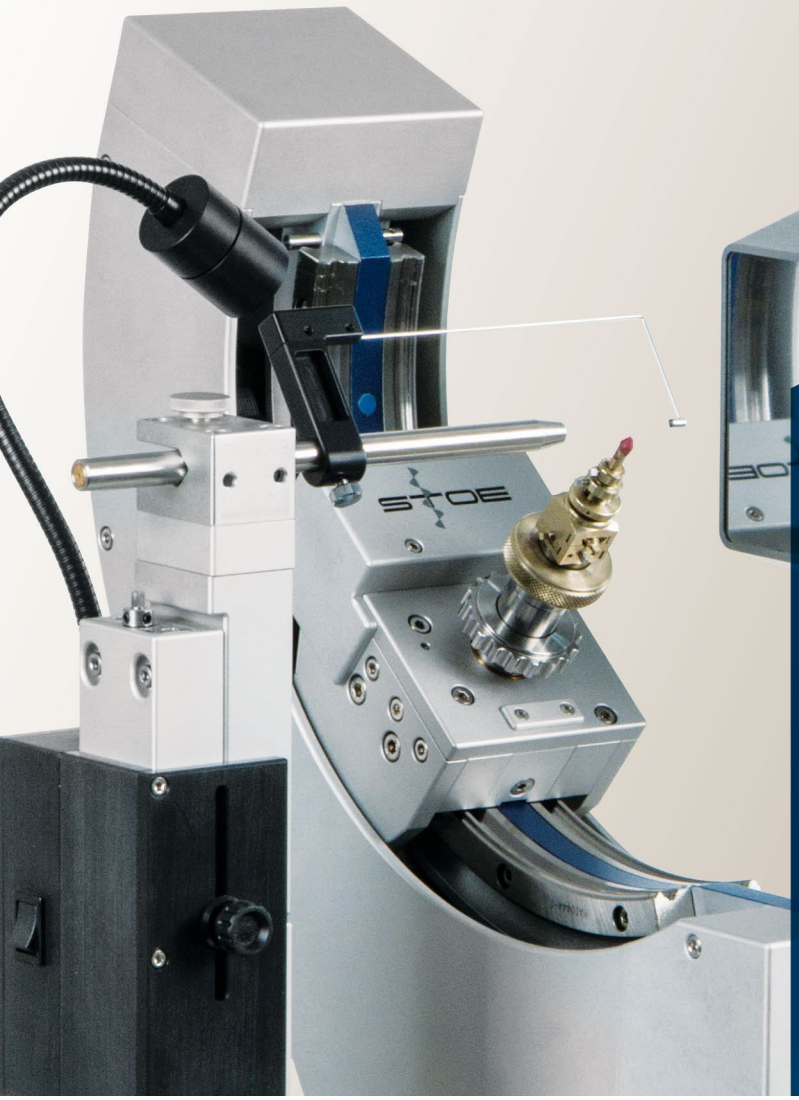
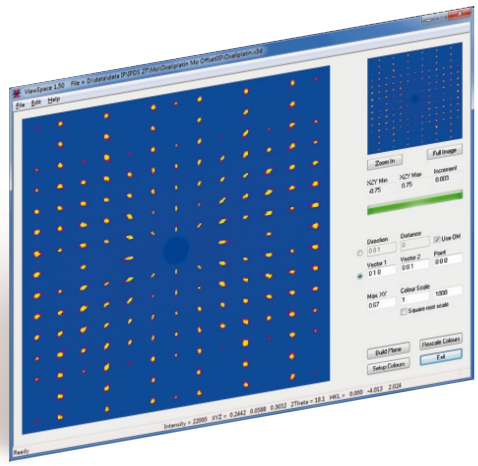
STOE

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
SINGLE CRYSTAL DIFFRACTION SOFTWARE

## DATA ACQUISITION

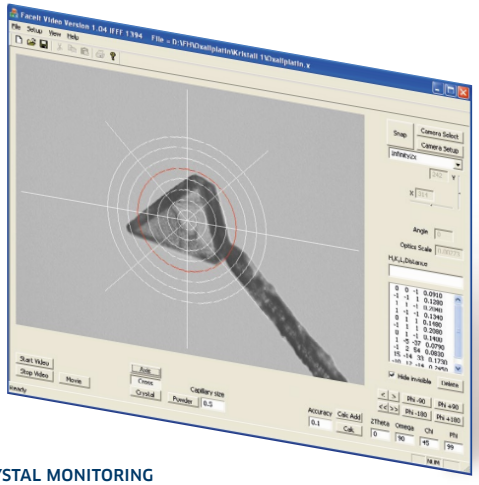
### INSTRUMENT CONTROL / MEASUREMENT / RUN OPTIMIZER

- 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

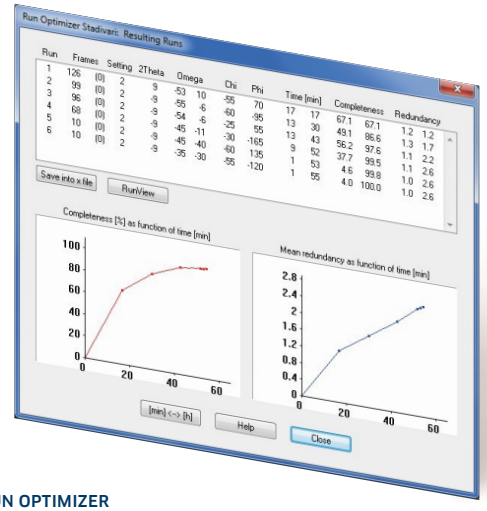
### FRAME GRAPHICS

- 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



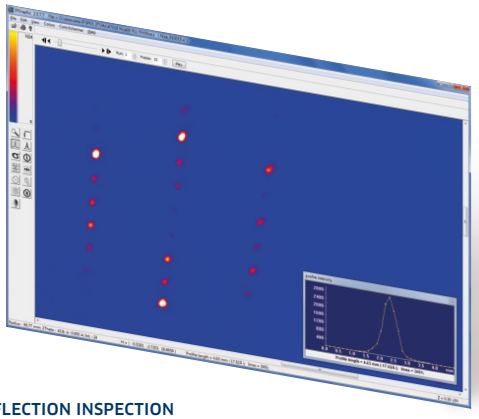
**CRYSTAL MONITORING**

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

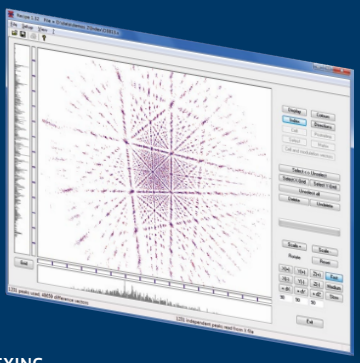
# IMAGE PROCESSING

## 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

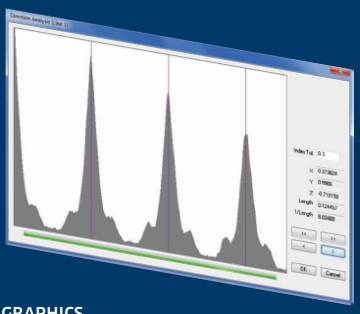
## INTEGRATION

- Use of elliptical reflection profiles and $\alpha_1/\alpha_2$-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



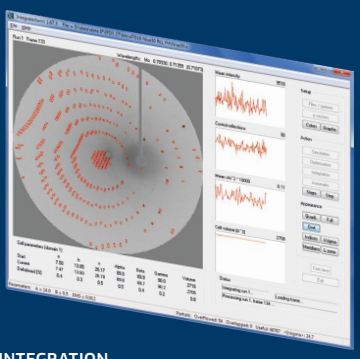
**ROBUST INDEXING**

Graphics supported indexing enables full control of the crystal quality



**CONTROL BY GRAPHICS**

During indexing, special effects as satellites may be detected easily

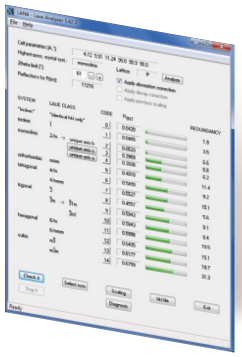


**REFLECTION INTEGRATION**

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”

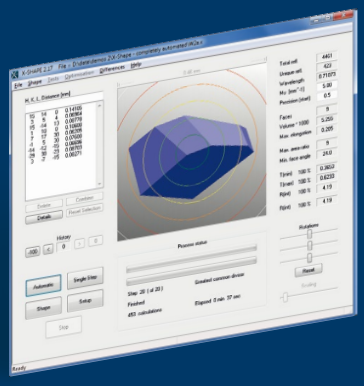


**LAUE ANALYZER**

Quick and easy check of the Laue group

# SINGLE CRYSTAL DIFFRACTION

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

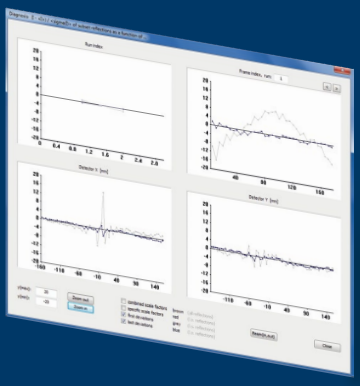
## CORRECTIONS

- 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

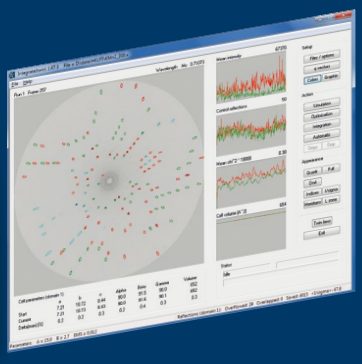
## EXTENDED ISSUES

### 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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