CrysAlisPro: New Features in Agilent's User-Inspired X-ray Crystallography Software Platform

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CrysalisPro has been designed to be as simple to use as possible:

- User friendly GUI
- Simple workflow
- Fully integrated platform
- Supporting SM and PX
- Highly automated......
- ...but full of manual features for those who want them
More than 30 Years of Innovation

1982
- Kuma launch First CCD
- Collaboration with Oxford Instruments

1995
- Oxford Diffraction formed
- Launch of Xcalibur diffractometer

2000
- First dual wavelength Gemini system
- Launch of Helijet Helium cooler
- Sapphire2- First Back illuminated CCD

2002
- First synchrotron CCD shipped to SNBL

2004
- Launch of higher intensity protein system
- Launch first sealed tube & multi-layer optics Protein system

2006
- CrysAlisPro software Launch
- Launched range of fast read out CCDs

2008
- First dual micro-source system

2010
- Reinvented Xcalibur & Gemini systems

2012
- New generation S2 CCD cameras

2014
- First Gradient Vacuum System
- Varian Inc. acquired by Agilent Technologies

Agilent Technologies
- Varian Inc. acquired by Agilent Technologies
X-ray Product Configurations
Modular Products - Tuned to Application

- 4-circle Goniometer
- X-ray Sources
- CCD Detectors
- Cryo-devices
Agilent S2 CCD Detectors

- Boost detector sensitivity by up to 50% with ‘Smart Sensitivity Control’
- Part of a unique Intelligent Measurement System, with flexible pixel binning
- Get better data up to 2x faster
What is ‘Smart Sensitivity Control’ SSC

- Smart Sensitivity Control allows for detecting very weak events!
- Like the ISO settings on digital cameras

These spots became visible only in high SSC mode!
SSC: Detective Quantum Efficiency (DQE)

\[
DQE = \frac{T_w \eta_{ph}}{1 + \frac{1}{g} + \frac{A(n_r^2 + i_d t)}{IT_w \eta_{ph} g^2}}
\]

Titan-S2 has roughly the sensitivity of Atlas, but with 50% larger area!
## Sample: Fe Formate

**Sample**: Fe formate  
**Size**: 0.1mm  
**Formula**: Fe C2 O6 H6  
**Cell**: 8.7 7.2 9.4 90° 97.5° 90°  
**SG**: P21/c  
**Instrument**: SuperNova  
**Wavelength**: Mo  
**Detector**: Titan S2  
**Detector distance**: 60 mm  
**Redundancy**: 10  
**Resolution**: 0.8Å  
**Exposure time**: 1.5s  
**I/sig**: 6  
**Total runs / frames (time)**: 11 runs / 762 frames (29min)
## Sample: Fe Formate

The same run list and exposure time for all measurements!

<table>
<thead>
<tr>
<th></th>
<th>2x2 binning</th>
<th>4x4 binning</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Standard SSC mode*</td>
<td>High SSC mode</td>
</tr>
<tr>
<td>I/sig</td>
<td>6.0</td>
<td>6.6</td>
</tr>
<tr>
<td>Rint</td>
<td>6.8%</td>
<td>5.6%</td>
</tr>
<tr>
<td>R1 (&gt;4sig(Fo))</td>
<td>3.27%</td>
<td>2.69%</td>
</tr>
<tr>
<td>R1 (for all data)</td>
<td>6.58%</td>
<td>4.87%</td>
</tr>
</tbody>
</table>

* Corresponds to Titan (previous generation) mode of operation

### 40% better!

[Agilent Technologies]
Sample: Fe Formate

Rint vs. resolution for different SSC modes
(Fe formate, 2x2 binning, I/sig=7, redundancy=10)
Agilent Logo Detector Sensitivity Test

Experimental Setup

X-ray source

Filter

X-ray detector
The filter has been chosen in such a way as to observe single photon events.

In order to visualize signal-to-noise differences 100 images are averaged and scaled so that the noise level is the same for all modes of operation.
## S2 Camera SSC Functionality

### 4x4 Binning

<table>
<thead>
<tr>
<th>Exposure time</th>
<th>0.5s</th>
<th>1s</th>
<th>2s</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Standard SSC mode</strong></td>
<td>![Image]</td>
<td>![Image]</td>
<td>![Image]</td>
</tr>
<tr>
<td><strong>High SSC mode</strong></td>
<td>![Image]</td>
<td>![Image]</td>
<td>![Image]</td>
</tr>
</tbody>
</table>

![Graph showing intensity over x-axis]
### S2 Camera SSC Functionality

#### 2x2 vs. 4x4 Binning

<table>
<thead>
<tr>
<th>Exposure time</th>
<th>0.5s</th>
<th>1s</th>
<th>2s</th>
<th>5s</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>2x2</strong></td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>4x4</strong></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
</tr>
</tbody>
</table>
Sample Ylid

- Equivalent result with half of exposure time!
- Thanks to flexibility of S2 detectors

<table>
<thead>
<tr>
<th></th>
<th>Titan S2, 2x2 binning, standard SSC mode*</th>
<th>Titan S2, 4x4 binning, high SSC mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure time</td>
<td>2 seconds</td>
<td>1 second</td>
</tr>
<tr>
<td>I/sig</td>
<td>5.3</td>
<td>4.3</td>
</tr>
<tr>
<td>Rint</td>
<td>9%</td>
<td>10%</td>
</tr>
<tr>
<td>R1 (&gt;4sig(Fo))</td>
<td>5.2%</td>
<td>5.24%</td>
</tr>
<tr>
<td>R1 (for all data)</td>
<td>8.2%</td>
<td>7.54%</td>
</tr>
</tbody>
</table>

* Corresponds to Titan (previous generation) mode of operation
Extremely Low Noise By Technology

- CCD are high gain integrative detectors
- Dark current is extremely low and stable
- Read noise is very low compared to the photon energy
- Extremely low noise level as observed from a 1 hour exposure (standard operation without X-rays): <0.1X-ray/pix/hr!

The image is displayed on the photon level.
Advances In Data Processing

- Improved data quality by novel approach to detector noise and X-ray background treatment
- Significant improvement in weak data quality

### Fe formate structure refinement results

<table>
<thead>
<tr>
<th></th>
<th>CrysAlisPro 171.36</th>
<th>CrysAlisPro 171.37</th>
</tr>
</thead>
<tbody>
<tr>
<td>I/sig</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Rint</td>
<td>5.4%</td>
<td>5.3%</td>
</tr>
<tr>
<td>R1 (&gt;4σ(Fo))</td>
<td>2.47%</td>
<td>2.42%</td>
</tr>
<tr>
<td>R1 (for all data)</td>
<td>4.45%</td>
<td>3.93%</td>
</tr>
</tbody>
</table>

CrysAlisPro 171.37 vs. 171.36 data processing results
Rint vs. resolution
(Fe formate, 4x4 binning, I/sig=7, redundancy=10)
Detective Quantum Efficiency (DQE) Advances

DQE versus intensity

DQE (KM4CCD, 2x2)

DQE for Mo radiation, peak dia 1mm at 60mm
Detective Quantum Efficiency (DQE) Advances

DQE versus intensity

DQE for Mo radiation, peak dia 1mm at 60mm

DQE (KM4CCD, 2x2)

DQE (Ruby, 2x2)
Detective Quantum Efficiency (DQE) Advances

**Detective Quantum Efficiency (DQE) versus intensity**

DQE versus intensity graph showing different detectors:
- **DQE (KM4CCD, 2x2)**
- **DQE (Ruby, 2x2)**
- **DQE (Atlas, 2x2)**

DQE for Mo radiation, peak dia 1mm at 60mm.
Detective Quantum Efficiency (DQE) Advances

DQE versus intensity

- DQE (KM4CCD, 2x2)
- DQE (Ruby, 2x2)
- DQE (Atlas, 2x2)
- DQE (Atlas-S2, 4x4 high SSC mode)

Detective Quantum Efficiency (DQE) for Mo radiation, peak dia 1mm at 60mm
Detective Quantum Efficiency (DQE) Advances

DQE versus intensity

DQE

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1

X-photons/reflection

1 10 100 1000 10000

DQE for Mo radiation, peak dia 1mm at 60mm

- DQE (Atlas-S2, 4x4 high SSC mode)
- DQE (Atlas, 2x2)
- DQE (Ruby, 2x2)
- DQE (KM4CCD, 2x2)
- DQE (CMOS detector)
## HW – Detector Tech: Read-Out Times

<table>
<thead>
<tr>
<th>Detector generation</th>
<th>Readout frequency for 1x1 binned image</th>
<th>Relative</th>
</tr>
</thead>
<tbody>
<tr>
<td>KM4CCD, Sapphire 1M</td>
<td>0.075Mhz</td>
<td>1</td>
</tr>
<tr>
<td>Ruby 4M</td>
<td>0.420Mhz</td>
<td>5.6</td>
</tr>
<tr>
<td>Atlas 4M</td>
<td>2.100Mhz</td>
<td>28</td>
</tr>
<tr>
<td>Atlas – S2 4M</td>
<td>4.400Mhz</td>
<td>56.7</td>
</tr>
</tbody>
</table>

State-of-the-art electronics provide:
- Speed
HW – Detector Tech: Read-Out Times

Duty cycle 0.22 s
Frames 1 2 3 4 5 6 7 8 9 10
Total time = 2.2 sec

Duty cycle 4.0 s
Frames 1 2 3 4 5 6 7 8 9 10
Total time = 40 sec
# HW – Detector Tech: Full Well/Dynamic

<table>
<thead>
<tr>
<th>Detector generation</th>
<th>Full well with respect to base binning pix (e⁻)</th>
<th>Relative</th>
</tr>
</thead>
<tbody>
<tr>
<td>KM4CCD, Sapphire 2x2</td>
<td>256’000</td>
<td>1</td>
</tr>
<tr>
<td>Ruby 2x2</td>
<td>128’000</td>
<td>0.5</td>
</tr>
<tr>
<td>Atlas 2x2</td>
<td>550’000</td>
<td>2.1</td>
</tr>
<tr>
<td>Atlas – S2 4x4</td>
<td>8’800’000</td>
<td>34.3</td>
</tr>
</tbody>
</table>

State-of-the-art electronics provide:
- Speed
- Instant binning switch
- Full well
New Binning Control

Binning and mode status now available all the time!
Intelligent Measurement System - IMS

- Powerful crystallographic sample recognition (cell, diffraction power, quality)
- Software combine possibilities of technology: binning, correlation, sensitivity, distance, scan width
- Optimal symmetry adapted strategy
- Optimal measurement pipeline and drive planning
- Implemented in CrysAlisPro 171.37
Optimization Of DC Parameters - IMS
Optimization Of DC Parameters - IMS

Note: Cumulative time now used instead of single frame time

If the user modifies one of the suggested settings, ‘Auto suggest’ link appears, which allows him to re-enable automatic suggestions.
Strategy 4.0

- Faster operation with pre-computed results
- Multi-core in all algorithms
- New experiment selection with higher data quality in mind: less and longer runs; better for scaling
## Strategy 4.0 – Multi-Core Speedup

- **4-core PC**

<table>
<thead>
<tr>
<th>Type of Cu Strategy</th>
<th>Orthorhombic</th>
<th>Monoclinic</th>
<th>Triclinic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Connectivity Mo, 0.8Å, 98.5%</td>
<td>5.4 -&gt; 4.2s</td>
<td>7.3 -&gt; 4.8s</td>
<td>9.4 -&gt; 5.7s</td>
</tr>
<tr>
<td></td>
<td>-22.0%</td>
<td>-34.0%</td>
<td>-40.0%</td>
</tr>
<tr>
<td>Charge density Mo, 0.4Å, 10 fold</td>
<td>12.5 -&gt; 6.1s</td>
<td>15.9 -&gt; 10.5s</td>
<td>17.5 -&gt; 13.8s</td>
</tr>
<tr>
<td></td>
<td>-51.0%</td>
<td>-34.0%</td>
<td>-21.0%</td>
</tr>
<tr>
<td>Absolute Config Cu, 0.78Å, 10 fold</td>
<td>8.3 -&gt; 5.3s</td>
<td>11.3 -&gt; 6.4s</td>
<td>17.9 -&gt; 8.4s</td>
</tr>
<tr>
<td></td>
<td>-36.0%</td>
<td>-43.0%</td>
<td>-53.0%</td>
</tr>
</tbody>
</table>
Strategy\(^4.0\) – Redundancy With Less Runs

- New experiment selection with **higher data quality in mind**: less and longer runs; better for scaling

<table>
<thead>
<tr>
<th>Type of Strategy 4 Redundancy runs</th>
<th>Orthorhombic</th>
<th>Monoclinic</th>
<th>Triclinic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge Density (Mo, 0.4 Å, 10 fold)</td>
<td>30→21</td>
<td>52→39</td>
<td>94→65</td>
</tr>
<tr>
<td></td>
<td>-30.0%</td>
<td>-25.0%</td>
<td>-30.9%</td>
</tr>
<tr>
<td>Absolute Config. (Cu, 0.84 Å, 10 fold)</td>
<td>25→22</td>
<td>38→37</td>
<td>69→64</td>
</tr>
<tr>
<td></td>
<td>-12.0%</td>
<td>-2.6%</td>
<td>-7.2%</td>
</tr>
<tr>
<td>Absolute Config. (Cu, 0.78 Å, 10 fold)</td>
<td>32→24</td>
<td>50→41</td>
<td>96→75</td>
</tr>
<tr>
<td></td>
<td>-25.0%</td>
<td>-18.0%</td>
<td>-21.9%</td>
</tr>
</tbody>
</table>
Typical Work-Flow

Mounting → Screen/Pre → Strategy → Experiment → Structure
Typical Work-Flow

- Mounting: <1min
- Screen/Pre: 10-60s → 1-15min
- Strategy: <30s
- Experiment: 15min-3d → concurrent
- Structure

Enabled by IMS
Simplified 3-Step Pre-Experiment Work-Flow

- Screens are not part of the experiment (no naming required)
- SM screens have a tab like PX screens
- Pre-exp (‘Plan experiment’) is launched from tab. Screens can be relauched.
- Pre-exp don’t require naming
- Strategy can name the experiment
Simplified 3-Step Pre-Experiment Work-Flow

- **Start/Stop:** Start new
  - **Exit**
  - **Screen**

- **F12**

- **Crystal Mounting Window**
  - **Next Crystal**
  - **Re-Image**
  - **Pre-exp.**

- **Screening Window**
  - **Sample info input**
  - **Strategy**

- **Pre-exp. Window**
  - **Sample info input**
  - **Screening Window**

- **Start/Stop:** Start new (no pre-experiment)
  - **Start/Stop:** Start new (no pre-experiment)

- **Strategy Window**
  - **Sample info input**

- **Main experiment**
  - **Strategy Window**
Tab Based Screening 1

**Well diffracting sample**

Diff. Limit: beyond 1.23 (theta res. limit) for I/sig=2.0
Mosaicity: c1=1.2, c2=1.2, c3=2.0 (deg), Iso=1.49 (deg)

**Experiment - Complete data for publication**

Name: exp_209

Detector=52.0mm, Res. = 0.837Ang, I/sig=15.0, width=1.0deg, Movie, cryo off. Strategy: Complete data (default mode). Exposure: 1.0s 40s

Exposure time: 1.0 s

**Goniometer**

Omega 20.0, Theta -35.0, Kappa 0.0, Phi 0.0, Distance 52.0

Generator: kV 50.0, mA 0.80
Tab Based Screening 2

SM Screening

Well diffracting sample

Experiment - Complete data for publication

Pre-experiment

Goniometer

Generator
Tab Based Screening 3

Shell command window (Ctrl - interrupts)

Command shell

DC PRE ACTION: Call PreExperiment Dialog (Init)
DC PRE ACTION: Init dialog
Collision check at 45.0 mm
Collision test: OK
DC PRE ACTION: New experiment name: exp_204
DC PRE ACTION: End init dialog
DC PRE ACTION: START button was pressed
Collision check at 45.0 mm
Collision test: OK
PREEXP4: changed run order 1 -> 0 (drive time 18 -> 10; already saved 8 [s])
PREEXP4: changed run order 5 -> 1 (drive time 18 -> 10; already saved 16 [s])
PREEXP4: changed run order 3 -> 2 (drive time 19 -> 10; already saved 17 [s])
PREEXP4: changed run order 5 -> 3 (drive time 19 -> 9; already saved 27 [s])
PREEXP4: changed run order 7 -> 6 (drive time 18 -> 13; already saved 32 [s])
PREEXP4: changed run order 8 -> 7 (drive time 18 -> 9; already saved 41 [s])

DC PRE ACTION: Experiment file name: exp_204
DC PRE ACTION: Write run list
DC PRE ACTION: Experiment detector distance: 45.00
DC PRE INFO: Experiment C:\<Path>\exp_204\pre_exp_204.run
DC PRE INFO: Expected chemical formula
DC PRE INFO: Interactive strategy after pre-experiment: 1
New ‘dc rrp’ or Finalization Dialog

- Now: Dialog with >10y history (old does not mean bad 😊!)
- Improvement: New dialog outline for SM and PX.
- Philosophy: Only required information is shown in order of importance
New ‘dc rrp’ Dialog

Old

New

Data reduction finalizing - rrp file to hkl file

Finalization dialog: SM experiment to hkl file

Sample

Empirical correction  
Numerical absorption  
Space group and AutoChem  
Filtrations and limits  
Output

[Images of data reduction and finalization dialogs]
New Finalizer – Popup Dialogs 1
New Finalizer – Popup Dialogs 2
New Finalizer – Advanced Abs Correction

1. Define crystal shape on movie
2. Tool for creating/modifying crystal shape without movie (face list)
3. Face based absorption method (dialog will shrink or expand depending on chosen method)
4. Settings for Gaussian grid method
5. Spherical absorption correction
All New ‘Data Finalizer’

- PX amino acid sequence tool
The point group -43m (cubic non-centro) was not handled correctly (Laue group was mapped to 432) and led to data artifacts when the second cycle in gral was not used or gral was entirely skipped.

The same is true for point groups ‘m’, 2mm, m2m, mm2, -4, 4mm, -42m, 31m, 3m1, -6, 6mm, -62m, -6m2
‘Abs Display’ Improvement’s

1. movie play buttons
2. Reciprocal and direct axis overlay
3. Face adjustment with d, h, k, l
4. small hkl's
5. max small hkl
6. display with small hkl
Data Reduction Of Overlapping Reflections (Twins/Multi-crystals)
Data Reduction Of Overlapping Reflections (Twins/Multi-crystals)
Twinning Integration Treatment – Overlap Threshold

0% overlap

100% Overlap

De-twinning attempted for structure solution

De-twinning not attempted

Changeable threshold
Twin Data Reduction
Current vs. New Approach

Current twin integration
- Component #1 PROFFIT
- Component #2 PROFFIT

Intensity decomposition during finalization

Less accurate HKLF4 and HKFL5 intensities

New simultaneous integration
Profile decomposition based on profile fitting of the overlapped area

More accurate profile-fitted HKLF4 intensity

Very accurate HKLF5 intensity

Twin finalization
Twinning
Integration Treatments – Smart Background

For datasets with uneven backgrounds, smart background can help.

From v37 upwards, smart background is now twin enabled
Twinning
Post Integration Treatments – Overlap Threshold

Version 36 or lower

Version 37 or higher
New Features

- Profile fitting
- Smart background (combination of local and average background)
- Bad-profile rejection filter
- Completeness-based reflection selection for HKLF4 file
Example 1

Xcalibur Nova (Cu), Atlas detector

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Data collection time</strong></td>
<td>20h 35min (2925 frames in 48 runs)</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>100K</td>
</tr>
<tr>
<td><strong>Cell</strong></td>
<td>5.45 6.15 25.3 87° 85.4° 72.9°</td>
</tr>
<tr>
<td><strong>Twin law</strong></td>
<td>2 components rotated 180° around c* axis</td>
</tr>
<tr>
<td><strong>Symmetry</strong></td>
<td>P-1</td>
</tr>
<tr>
<td><strong>Overlapping statistics</strong></td>
<td>Twin ratio 80:20</td>
</tr>
<tr>
<td></td>
<td>49% isolated,</td>
</tr>
<tr>
<td></td>
<td>44% partially overlapping,</td>
</tr>
<tr>
<td></td>
<td>7% fully overlapping</td>
</tr>
<tr>
<td></td>
<td>reflections</td>
</tr>
</tbody>
</table>
## Example 1

![Molecular Structure Image]

<table>
<thead>
<tr>
<th></th>
<th>HKLF4</th>
<th>HKLF5</th>
<th>Relative Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Old</td>
<td>New</td>
<td></td>
</tr>
<tr>
<td>Rint</td>
<td>3.2%</td>
<td>4.4%</td>
<td>-</td>
</tr>
<tr>
<td>Completeness</td>
<td>82%</td>
<td>82%</td>
<td>100%</td>
</tr>
<tr>
<td>R1 (Fo &gt; 4sig(Fo))</td>
<td>7.1%</td>
<td>5.6%</td>
<td>-22%</td>
</tr>
<tr>
<td>R1 for all data</td>
<td>7.5%</td>
<td>6.3%</td>
<td>-16%</td>
</tr>
<tr>
<td>Highest peak</td>
<td>0.28</td>
<td>0.24</td>
<td>-0.28</td>
</tr>
<tr>
<td>Deepest hole</td>
<td>-0.28</td>
<td>-0.25</td>
<td>-0.25</td>
</tr>
</tbody>
</table>
Example 2

<table>
<thead>
<tr>
<th>Xcalibur (Mo), Eos detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data collection time</td>
</tr>
<tr>
<td>Temperature</td>
</tr>
<tr>
<td>Cell</td>
</tr>
<tr>
<td>Twin law</td>
</tr>
<tr>
<td>Symmetry</td>
</tr>
</tbody>
</table>
| Overlapping statistics      | Twin ratio 54:46  
74% isolated,  
21% partially overlapping,  
5% fully overlapping reflections |
### Example 2

<table>
<thead>
<tr>
<th></th>
<th>HKLF4</th>
<th>HKLF5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Old</td>
<td>New</td>
</tr>
<tr>
<td>Rint</td>
<td>10.5%</td>
<td>8.2%</td>
</tr>
<tr>
<td>Completeness</td>
<td>92%</td>
<td>91%</td>
</tr>
<tr>
<td>R1 (Fo &gt; 4sig(Fo))</td>
<td>6%</td>
<td>3.02%</td>
</tr>
<tr>
<td>R1 for all data</td>
<td>7.62%</td>
<td>4.23%</td>
</tr>
<tr>
<td>Highest peak</td>
<td>4.49</td>
<td>1.84</td>
</tr>
<tr>
<td>Deepest hole</td>
<td>-4.42</td>
<td>-1.24</td>
</tr>
</tbody>
</table>
### Example 3

**SuperNova (Cu), Atlas detector**

<table>
<thead>
<tr>
<th>Data collection time</th>
<th>1h 19min (77 frames in 1 run)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>100K</td>
</tr>
<tr>
<td>Cell</td>
<td>45.4 51.2 80.9 90 90 90</td>
</tr>
<tr>
<td>Twin law</td>
<td>2 components rotated by -138.6° around -0.35 0.84 -0.41 (rec) axis</td>
</tr>
<tr>
<td>Symmetry</td>
<td>P2₁2₁2₁</td>
</tr>
<tr>
<td>Overlapping statistics</td>
<td>Twin ratio 54:46</td>
</tr>
<tr>
<td></td>
<td>30% isolated, 65% partially overlapping, 5% fully overlapping reflections</td>
</tr>
</tbody>
</table>
Example 3

- 95% of the reflections can be de-convoluted to serve as an input to MTZ.

<table>
<thead>
<tr>
<th>HKLF4</th>
<th>Old</th>
<th>New</th>
</tr>
</thead>
<tbody>
<tr>
<td>inf-4.50</td>
<td>0.043</td>
<td>0.03</td>
</tr>
<tr>
<td>4.50-3.56</td>
<td>0.062</td>
<td>0.043</td>
</tr>
<tr>
<td>3.56-3.12</td>
<td>0.095</td>
<td>0.072</td>
</tr>
<tr>
<td>3.12-2.84</td>
<td>0.137</td>
<td>0.095</td>
</tr>
<tr>
<td>2.84-2.65</td>
<td>0.182</td>
<td>0.116</td>
</tr>
<tr>
<td>2.65-2.49</td>
<td>0.223</td>
<td>0.136</td>
</tr>
<tr>
<td>2.49-2.37</td>
<td>0.266</td>
<td>0.167</td>
</tr>
<tr>
<td>2.37-2.27</td>
<td>0.31</td>
<td>0.207</td>
</tr>
<tr>
<td>2.27-2.18</td>
<td>0.387</td>
<td>0.244</td>
</tr>
<tr>
<td>2.18-2.10</td>
<td>0.406</td>
<td>0.272</td>
</tr>
<tr>
<td>Overall</td>
<td>0.129</td>
<td>0.089</td>
</tr>
</tbody>
</table>
## Further Trials

<table>
<thead>
<tr>
<th>Data set</th>
<th>Structure refinement R1 (HKLF5)</th>
<th>Relative improvement to the old method</th>
<th>Overlapping reflections statistics</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Old integration</td>
<td>New integration</td>
<td>Isolated</td>
</tr>
<tr>
<td>Werner Massa</td>
<td>3.28%</td>
<td>2.34%</td>
<td>-29%</td>
</tr>
<tr>
<td>Zn_Bron (Pomiar4c_100K)</td>
<td>4.79%</td>
<td>4.13%</td>
<td>-13%</td>
</tr>
<tr>
<td>MC008</td>
<td>6.05%</td>
<td>5.07%</td>
<td>-15%</td>
</tr>
<tr>
<td>Pol530</td>
<td>6.36%</td>
<td>5.47%</td>
<td>-14%</td>
</tr>
<tr>
<td>Second_crystal_100k</td>
<td>3.29%</td>
<td>2.54%</td>
<td>-22%</td>
</tr>
<tr>
<td>Bn_pncuminb</td>
<td>3.97%</td>
<td>3.22%</td>
<td>-18%</td>
</tr>
<tr>
<td>Twin_2</td>
<td>3.95%</td>
<td>2.75%</td>
<td>-31%</td>
</tr>
<tr>
<td>spingler</td>
<td>7.01%</td>
<td>5.43%</td>
<td>-23%</td>
</tr>
<tr>
<td>cmx53</td>
<td>5.36%</td>
<td>4.08%</td>
<td>-24%</td>
</tr>
<tr>
<td>Byu12</td>
<td>4.66%</td>
<td>4.45%</td>
<td>-5%</td>
</tr>
<tr>
<td>cmx45</td>
<td>6.39%</td>
<td>5.89%</td>
<td>-8%</td>
</tr>
<tr>
<td>Pol411</td>
<td>11.61%</td>
<td>10.18%</td>
<td>-12%</td>
</tr>
<tr>
<td>Pol426</td>
<td>16.35%</td>
<td>15.04%</td>
<td>-8%</td>
</tr>
<tr>
<td>Pol312</td>
<td>14.07%</td>
<td>13.22%</td>
<td>-6%</td>
</tr>
</tbody>
</table>
Automatic Multi Scenario Data Processing

- xx profitloop
- Some 32+ processing combinations
External Frame & File Formats

CrysAlisPro can process frames from most detector manufacturers

This includes:

- Simple tools for importing frames
- Esperanto feature for defining new frame formats
- These features are ideal for processing synchrotron data
- Data can also be exported in various file formats for use in other programs, such as Jana
Esperanto generator

dc rit: Diamond ID 19 - Dectris 300k turned

- Command **dc rit**
- Use of known format dectris. Header values are read.
- Camera turned 270deg. Non-square detector is padded by zeros.
- The header scan values are wrong by 3% (Scan scale err 0.97)
- Then esperanto createrunlist
- Slight play in Ewald$^\text{Pro}$ to get the center right.
- The several cycles to refine instrument model.
XX Gandolfi: Powder Patterns From Single Crystal Experiments

- Gandolfi method images a single crystal on film as powder diagram
- You can do the same using a single crystal data set and doing a powder pattern extraction.
- The difference to a normal powder extraction is: background subtraction before image accumulation. The results are striking!
- Now you can deposit new mineral structures with experimental powder pattern extracted from your single crystal data! A super sensitive Gandolfi camera.
- See also issue 81: ITS 81 XX GANDOLFI - Background computations for powder analysis
2-Tube Stand-By

- Quickens lamp switching for service
- Slightly increases unused tube temperature and helps fight condensation
- Increase tube lifetime
- Remove need for conditioning

Available for SuperNova dual systems
Email Feature

- Normal and Admin users
  - Normal users can get info on their experiment
    - Pre/experiment results
    - Laue change
    - Door open ...
  - Admins get admin related infos on every experiment of all users
    - Par file change
    - User change
    - Tube life time (one time events)
    - Flow rates
Support Ag Wavelength

- Ag wavelength is now supported for SuperNova instruments
- All aspects of the GUI and software are Ag aware:
  - Calibration
  - Strategy
  - Generator device control
Source flexibility - Silver

\[ \lambda = 0.55941 \text{ Å} \]
Source flexibility - Silver

- Useful applications include
  - High Pressure
  - Charge Density
  - Highly-absorbing samples
Support Of Helix Cooler

- As a SuperNova dual special now the Oxford Cryosystem Helix is supported with a roof holder
- Special microscope added
- Special collision model
- Co-mounting of Helix and Cryo possible
- Odbench support of Helix
CrysAlis**Pro** help

Version presentations - Embedded pdf files

- Version presentations
- PDF links. Some 200+ presentation pages…

**New features in 171.37 - Overview**

Dear CrysAlisPro users!

Also version 37 includes a presentation of new features. To see a graphic presentation is added here. A lot of our new features are presented here. Our contact people at shows, visits, user meetings, the web and xrssoftware@agilent.com have helped to distill a list of features the users.

Here are some quick links to relevant topics:

- Simultaneous twin integration
- Data reduction
- New CCD cameras - S2
- Data collection
- Strategy
- Hardware/Instrumentation
- CSD and local data base
- Misc

Here you can access the version news:

- Simultaneous twin integration
- Data reduction
- New CCD cameras - S2
- Data collection
- Strategy
- Hardware/Instrumentation
- CSD and local data base
- Misc

**171.37 - Simultaneous twin integration**

- New simultaneous twin integration

More accurate profile-fitted HKLF4 intensity

Less accurate HKLF4 and HKLF5 intensities

Comparison of old and new twin integration

The version 37 features a new integration algorithm for twins. So far the twin components were treated/integrated in separate passes. As each pass did not know about other twin component it yield sub-optimal results. Version 37 now has a simultaneous twin integration, which yield more accurate results on HKLF4 and HKLF5 processing. On the twin finalizer we replaced the rather cryptic overlap parameter with target completeness as to simplify the meaning for the users.

Please go through the attached presentation for more details about twin processing. Twin Data Processing in CrysAlisPro version 37. The pdf will give you a detailed Powerpoint presentation on the features and tools included.

**Features**
CrysAlis Pro 171.37.33
Currently under release test

- Ewald Pro with CSD links for multi-crystals
- Ewald Pro with ‘Collapse view’
- Center finding
CrysAlisPro 171.37.33

- Unwarp browse
- Shape optimization reworked
- Embedded pdfs better high-lighted
Software Updates

- **CrysAlisPro** is frequently updated with fixes for known problems
- New features are introduced in annual major updates
- All updates are **Free** and available from our user forum, www.agilentxrdforum.com
- **Free** multi-user, multi-site license
The IUCr ‘Crystallography in Everyday Life’ Photo Contest
Win one of two $1,000 bursaries to attend the IUCr Congress, Montreal in August 2014

IUCr-UNESCO Open Labs
Supporting IYCr2014 Open Lab projects across the globe

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www.agilent.com/chem/iycr2014
Find out more at:

www.agilent.com/chem/xrd