Poster

Open the black box with X-Area's intuitive, interactive, and colourful data quality assessment graphics.

L. C. Folkers[1], F. Hahn[1], J. Richter[1]

[1]*STOE & Cie GmbH, Hilpertstrasse 10, 64295 Darmstadt, Germany*

folkers@stoe.com

Are your crystals ever as perfectly round as theory assumes the perfect crystal to be, never twinned, never strongly absorbing, never seeing any icing on your frames? In real life, such perfection is rarely met, and every measurement requires a unique data processing treatment. Making an informed decision on a data processing strategy can be difficult when results are not becoming visible before the end of a refinement.

X-Area features the "DIAGNOSIS", "PLOTS", "TWIN PLOTS" and "SPHERES" graphical subprograms of the Laue Analyzer (LANA) which exhibits the impact of data processing directly after it has been applied. These modules facilitate tracking normalized deviations of reflection groups, for example, across frames (Fig. 1). Thus, an unusual number of strong deviations of the normalized intensity can immediately be caught.

The most recent addition to these programs is called "SPHERES" and presents a visually intuitive quality evaluation (Fig. 2). Utilizing color-coded representations, it assesses the quality of incident and reflected beam scaling, total scale factors, and the changes in the reflected beam deviations, which is an elegant and easily accessible way to monitor the scaling progress.

In this talk we will introduce on examples how these graphical tools give the user readily comprehensible information about the quality of their data processing and thus can prevent falsely assigned elements or odd ADP shapes *before* spending valuable time on the refinement.

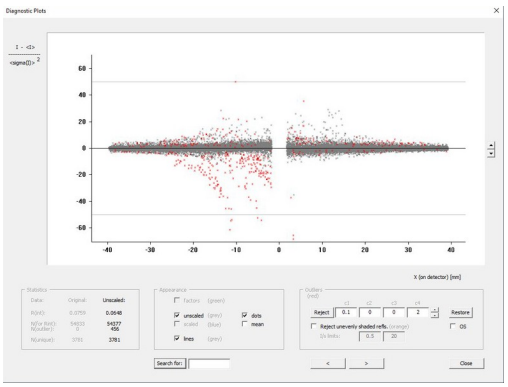

Figure 1. Effects of inadequate data treatment visible in the large number of reflections with strongly negative normalized deviation. The origin of this behavior will be discussed in the talk.

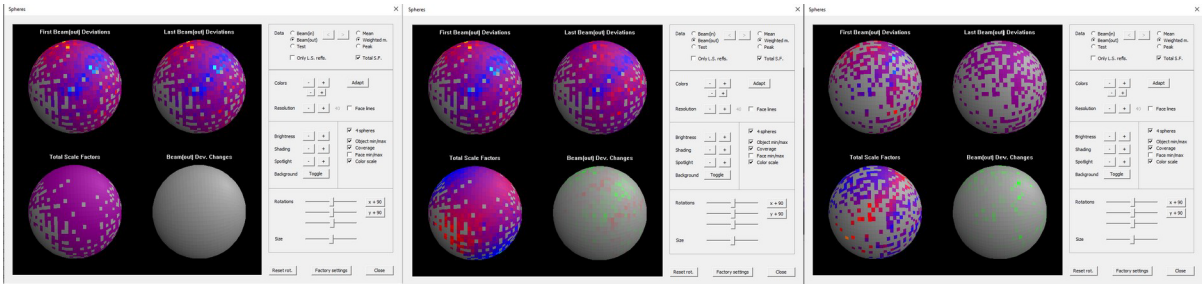

Figure 2. Data Spheres of a sample before (A), after light frame and reflected beam scaling (B), after stronger frame and reflected beam scaling and outlier rejection (C).