DETECTOR METROLOGY TOLERANCE IN CXI64813

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During our data analysis of experiment cxi64813, conducted by the Doniach group in January 2013, we discovered that obtaining a very precise detector geometry was necessary for the success of our experiment. The main source of difficulty was the mobile quads on the DS1 CSPAD at CXI – no information about the relative position of these quads is currently provided by LCLS, leaving it up to the user to optimize their position.

We have optimized the detector metrology based on a calibration sample of gold nanoparticles, which when illuminated with the LCLS beam generate two strong powder rings on the detector (Fig. 1). In addition to optimizing the detector metrology, collecting data on this sample at many detector positions allowed us to calibrate the distance from our sample to the detector and also the beam energy – these were found to differ from the values reported by online instrumentation at CXI by 1.17 mm and 82 eV (average), respectively. The code to perform geometry optimizations and energy/distance calibration is simple to use and is publicly available at: `https://www.github.com/tjlane/pypad`.

The following report details what we discovered and hopefully provide insight into how to provide a higher-quality metrology for users. This is critical for experiments like ours that are especially sensitive to the detector metrology. As a guiding principle, an optimal scheme would provide the metrology with a tolerance than a single pixel ($< 100\mu$m). We suspect this will be generally acceptable for all experiments.

Effect of Metrology Error on the Experiment. Here, I detail how small errors in the metrology affect our experiment. We are interested in computing intensity correlation functions, specifically

$$C(q_1, q_2, \Delta) = \langle \delta I(\mathbf{q}_1)\, \delta I(\mathbf{q}_2) \rangle_{\{\text{shots}\}}$$

with $I(\mathbf{q})$ the intensity measured at scattering vector $\mathbf{q}$, and δ indicates the fluctuations around the mean.

We assessed the error introduced in these measurements by computing the correlation function for our data on our optimized metrology in addition to a series of perturbed metrologies, where the quads on the CSPAD were shifted in a way so as to emulate the dilation of the central hole present in the CXI DS1.

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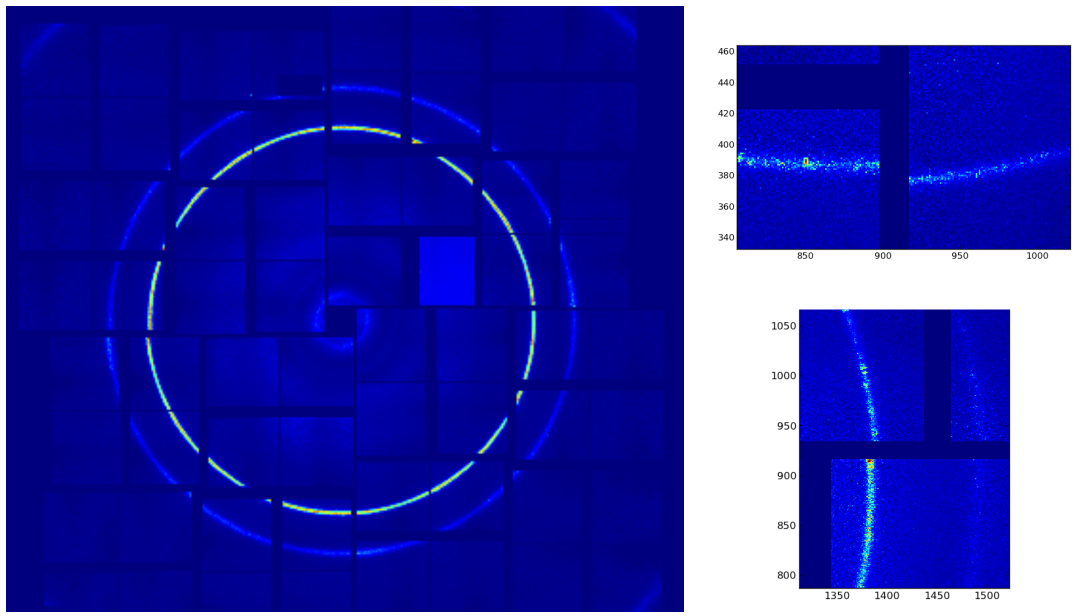

FIGURE 1. The gold calibration sample used (r0135) for cxi64813. Left, the optimized geometry showing the two rings used to optimize the metrology. Right, snapshots of the metrology provided by LCLS, showing errors in the relative positions of the quads.

To assess the error, we introduce the total relative error (TRE), defined for dilation d as

$$TRE(d) = \sum_{\Delta} \left| \frac{C(q_1, q_2, \Delta)|_d - C(q_1, q_2, \Delta)|_{d=0}}{C(q_1, q_2, \Delta)|_{d=0}} \right|$$

The TRE provides a normalized measure of the difference between correlation functions measured from two different metrologies. Intuitively, one can think of this quantity as the average percent error across all points Δ that constitute the correlation function.

Figure 2 reports the TRE as a function of dilation from the optimal metrology at $d = 0$. It is clear that even for small perturbations ($d = 250\mu$m) the TRE exceeds unity, meaning there is an average of greater than 100% error in most values of the correlation function. The situation isn't quite as bad as that number might indicate, since the TRE is dominated by values of the correlation function near zero. Figure 2 also shows the correlation functions themselves, and one can see the qualitative nature of those functions change a bit slower, but are clearly different by eye for dilations of 500μm.

One should note that the correlation functions shown here are almost entirely due to the response of the CSPAD itself – the signal from the sample is much smaller and likely more sensitive to the detector geometry. At this time extracting this experimental signal is an ongoing research project so is not discussed here.

Based on these measurements, we estimate that metrologies that achieve a precision of 100μm or better should be sufficient to be sure that detector metrology is not a limiting factor in the quality of results we can obtain at LCLS.

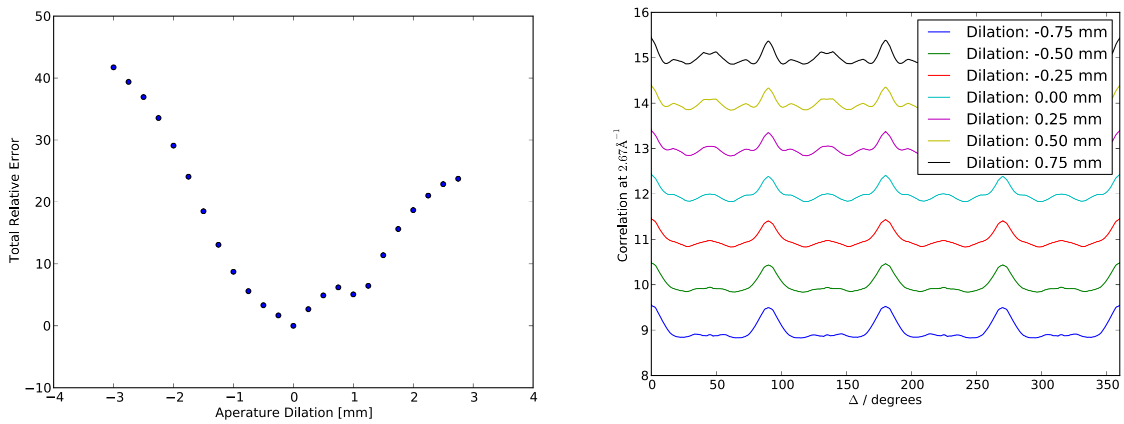

Figure 2. Right: TRE as a function of the size of the central hole in the LCLS camera. The Left: The correlation functions at positions around the optimal metrology at dilation $d = 0$.

Quality of Optical Metrologies. During our optimization of the detector geometry, we noticed that in a small number of cases the optical metrology contains errors larger than it should given the precision of the optical microscope. We are currently comparing the angle between the rectangular sides of each two-by-one, and ensuring this angle is near 90°. The longest two-by-one side is 388 pixels long. Therefore to achieve single-pixel accuracy in the metrology, the angle between the two two-by-one sides should be less than

$$\theta = \arctan\left(\frac{1\text{ px}}{388\text{ px}}\right) \approx 0.148^\circ$$

The majority of two-by-ones pass this check, but for instance in the most recent CXI DS1 metrology, two-by-one 0 on quad 2 failed with an angle $\theta = 0.482^\circ$.

That said, the fact that the metrology is good to within a pixel for the majority of two-by-ones means that it is precise enough for our experiment.

Wish List from the User. In conclusion, I present a list of wishes from the user's view point that can help guide the development of the next generation of metrology techniques and technology. It would be great if there were a metrology scheme that was:

(1) able to completely specify/restrain geometry to within 100μm tolerance.

(2) applicable for all detector/aperture motor positions, not dependent on motor readouts.

(3) had minimal intervention in experiment; no scattering from the setup, small number of pixels affected.

(4) employed minimal user time to obtain a geometry. LCLS time is precious! Less than 1 hour is acceptable.

(5) simple to implement and robust to different experimental setups.

(6) supported by quality software.

Any system that meets these needs should be sufficient for nearly all user's needs. Current ideas as to how to achieve these goals include:

(1) extending the optical metrology to also measure the relative positions of the quads.

(2) introducing some sort of shadow-casting object into the chamber that allows the determination of the relative positions of the quads.

Done right, either of these ideas may fit the bill.

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Feel free to contact me if I can be of any help: `tjlane@stanford.edu`.