Supplemental Information: Computer Assisted Area Detector Masking

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1 Detector Q resolution

Figure 1 shows the geometry of x=ray scattering onto a flat image plate detector.

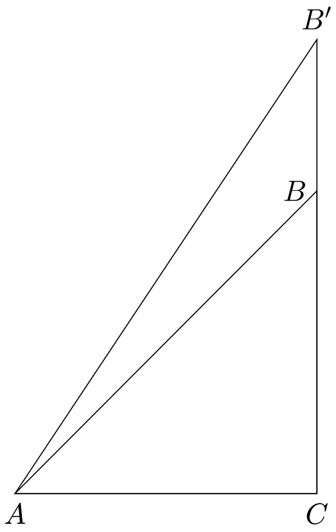

Figure 1: Scattering onto a flat detector

2 Simulated Data Mask Generation

In the case of the simulated data four systems were created: 1) dead/hot pixels with varying numbers of defective pixels, 2) dead/hot pixels on a corner-centered detector, 3) beamstop holder with varying beamstop holder transmittance, 4) rotated beamstop holder with varying beamstop holder transmittance, The base scattering was produced by

$$I = 100\cos(.1Q)^2 + 150 \tag{1}$$

where Q is a pixel's distance from the beam point of incidence. While this scattering is not the most accurate representation of x-ray scattering it provides a good foundation, showing the effectiveness of the masking with ideal data. The positions of the dead/hot pixels were chosen at random as was the dead or hot nature of the defect. Dead pixels had values from 0 to 10, while hot pixels had values from 200 to 255. The beamstop was positioned at the vertical center of the detector with an initial width of 60 pixels and final width of 120 pixels. The height of the beamstop was 1024 pixels. The beamstop was calculated to attenuate the x-ray scattering signal at various transmittance, as various beamstop holder materials have different transmittance.

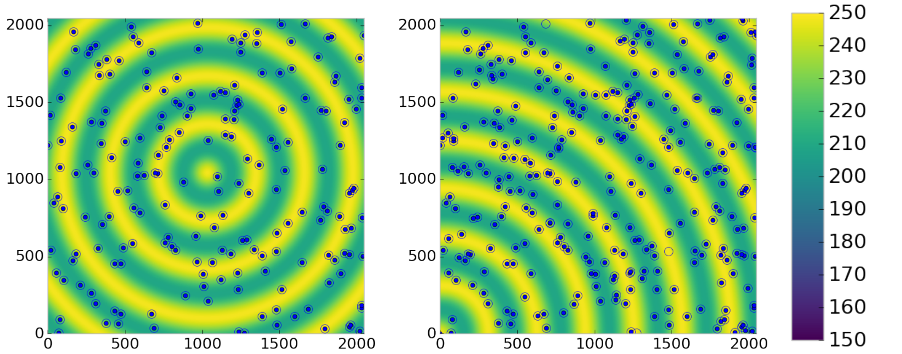

Figure 2: Generated dead/hot pixel masks for a detector with bad pixels. left: auto-mask with a centered beam with 200 bad pixels and right: auto-mask with off centered beam with 300 bad pixels. The bad pixels are noted with open circles, masked pixels are noted with solid circles.

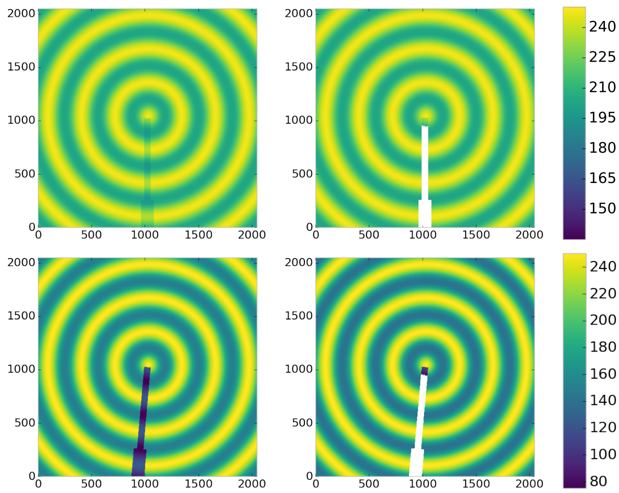

Figure 3: Generated beamstop masks. top: mask for a beamstop holder with 90%, transmittance. Bottom: mask for an off axis beamstop with 50% transmittance, left: the raw image, right: the masked image. Note that the masked pixels in the middle are white.

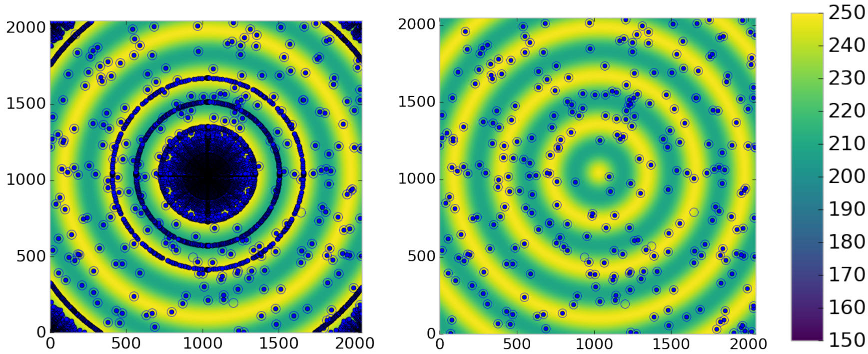

Figure 4: Generated dead/hot pixel masks for a detector with 300 bad pixels. left: the standard even bin mask and right: the Q resolution binned mask. The bad pixels are noted with open circles, masked pixels are noted with solid circles.

3 Results and Discussion

3.1 Simulated Examples

Three main studies were run each examining a different aspect of the simulated or experimental studies. These included, masking bad pixels, masking a beamstop holder, and masking experimental data. Figures 2 and 3 show the results of the masking algorithm on simulated images.

Figure 2 indicates that the masking algorithm masks the image almost perfectly, with very few missed bad pixels or good pixels masked. The centered mask had an average, over 10 runs, of 6.5 (0.022%) false negatives and 0.0 false positives, while the off center mask had 5.6 (0.019%) false negatives and 7.0, (0.023%) false positives. With standard threshold masking the threshold must be set for the entire detector, either leaving some bad pixels unmasked or removing good pixels. The localized nature of the ring based masking eliminates this issue as the threshold is different for each ring according to its scattering. Thus, pixels at strongly scattering angles are not masked out if they have similar values to hot pixels at low intensity angles, thus preserving more usable data.

The beamstop holder masks shown in figure 3, show similar results across the transmittance range, missing only a small part of the beamstop holder near the point of incidence. This close to the center of the detector the beamstop holder becomes a statistically significant part of the total number of pixels in a given ring, thus it can not be masked out using a statistical search of the rings. For most PDF and XRD studies this small area can be masked automatically by masking all the pixels who's distance from the point of incidence is smaller than a given radius r, or can be neglected outright as the area is not used in the analysis or refinement.

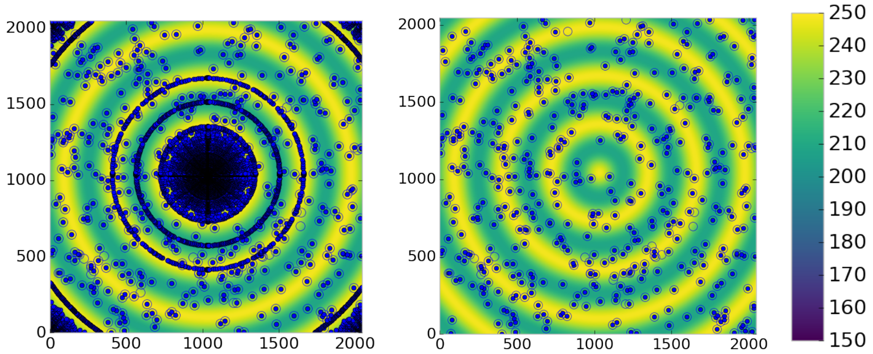

Figure 5: Generated dead/hot pixel masks for a detector with 500 bad pixels. left: the standard even bin mask and right: the Q resolution binned mask. The bad pixels are noted with open circles, masked pixels are noted with solid circles.

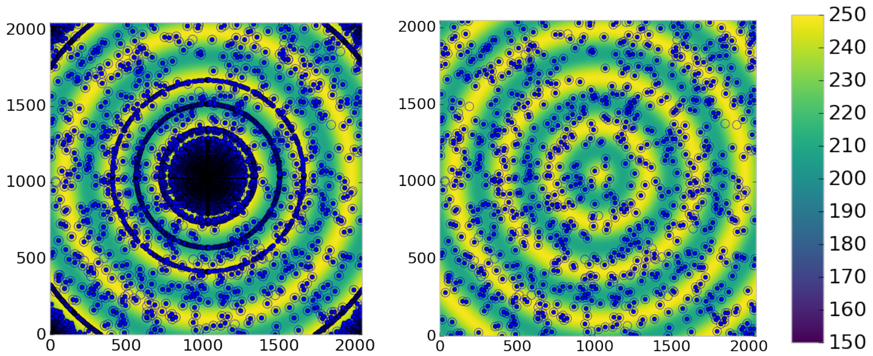

Figure 6: Generated dead/hot pixel masks for a detector with 1000 bad pixels. left: the standard even bin mask and right: the Q resolution binned mask. The bad pixels are noted with open circles, masked pixels are noted with solid circles.

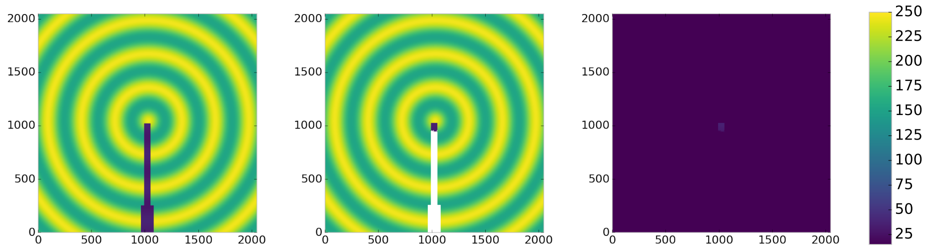

Figure 7: Generated beamstop holder masks for a beamstop holder with 10% transmittance. left: the raw image, middle: the masked image, and right: the missed pixels. Note that the masked pixels in the middle are white.

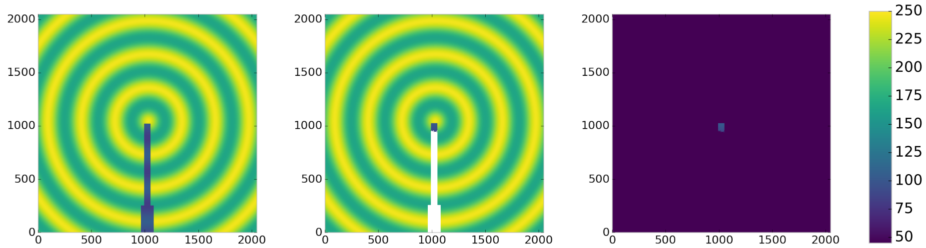

Figure 8: Generated beamstop holder masks for a beamstop holder with 30% transmittance. left: the raw image, middle: the masked image, and right: the missed pixels. Note that the masked pixels in the middle are white.

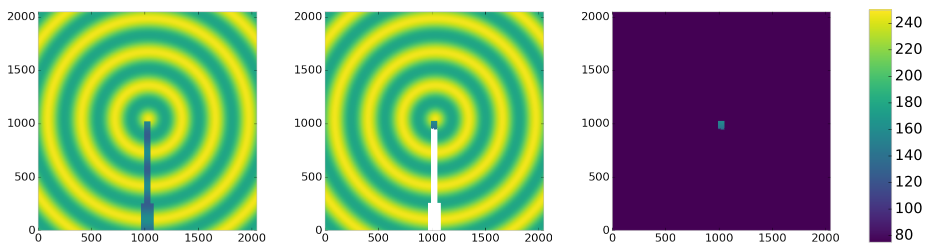

Figure 9: Generated beamstop holder masks for a beamstop holder with 50% transmittance. left: the raw image, middle: the masked image, and right: the missed pixels. Note that the masked pixels in the middle are white.

Figures 4 - 9 show additional masks created for simulated images with more bad pixels and beamstops with less transmittance.