Correcting Spatial Distortions and Nonuniform Response in Area Detectors

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Abstract

Software and hardware methods have been developed to correct images for spatial and intensity distortions produced by optical and electro-optical components in X-ray area detectors. Spatial distortions are divided into two types: gross distortions produced by the inherent properties of the detector components and local distortions formed by irregularities in the components. Intensity distortions are separated into three types: those caused by background nonuniformity; those resulting from pixel-dependent nonuniform intensity response; and those resulting from time-dependent variations in background and incident-beam intensity. From background, flat-field, reference and mask images, ‘forward’ and ‘reverse’ interpolation tables are generated to correct for spatial distortions and a lookup table is generated to correct for nonuniform sensitivity. The routines have been used successfully on four different area detectors to correct entire images or to correct intensities of individual Bragg peaks. The spatial-distortion correction is good to within 0.1 pixels and the nonuniformity correction to <2%.

Introduction

Electronic area detectors exhibit spatial distortions and nonuniform sensitivity response introduced by optical and electro-optical components. Because it would be impractical to eliminate most distortions and nonuniformities by designing specialized hardware, they must be corrected in software. The distortions present in most electronic area detectors require correction if quantitative results are desired. As long as the detector response is time-independent and can be accurately modeled in software, the corrections need not introduce any additional uncertainties in the data.

Device-specific spatial-distortion correction routines have been developed for the commercially available detector systems. For the Xentronics detector system, corrections are based either on linear interpolations (Durbin, Burns, Mulai, Metcalf, Harrison & Wiley, 1986) or a Fourier series (Kabsch, 1988). Routines developed for the FAST system utilize a bivariate power-series expansion (Thomas, 1989). These methods, which were developed for specific instruments, can be difficult to adapt to other detector systems. Our approach has been to develop a general calibration method that (a) has algorithms based on the optical characteristics of detector components, (b) works with several types of detectors, (c) is straightforward to apply and (d) introduces errors smaller than other experimental uncertainties in the data.

Our method for correcting geometric distortions is based on the combination of a radial function to model the gross distortions and a two-dimensional interpolation matrix that describes local distortions. We assume that all geometric distortions are smoothly varying on the scale of a pixel. In vidicon and CCD-based detectors such as the FAST, Brandeis SIT and Argonne CCD detectors, radial (pin-cushion) geometric distortion of the image is introduced by the inverting electrostatic image intensifier(s) (Arndt, 1985; Kalata, 1985; Strauss, Westbrook, Naday, Coleman, Deacon, Travis, Sweet, Pflugrath & Stanton, 1990). The Siemens multiwire detector also has radial (barrel) distortion produced by field lines at the detector window (Derewenda & Helliwell, 1989). These detectors and other detectors without inherent radial distortions, such as the San Diego Multi-Wire (SDMW) (Hamlin, Cork, Howard, Nelson, Vernon, Matthews, Xuong & Perez-Mendez, 1981) and Brandeis CCD (Kalata, Phillips, Stanton & Li, 1990), still have local geometrical distortions introduced by fiber-optic tapers and plates, lenses, nonuniform field lines and the geometry of the sensor. Geometric distortion from an inverting image intensifier is ~8% at the edge of the field. Local distortions in fiber-optic tapers are typically ~1–2% from a straight line.

Variations in response over the active area occur in all detector systems. These variations can be separated into three components: background, nonuniform intensity response and time-dependent changes. (We assume the response of each pixel is a linear function of the number of incident X-ray photons.) The background is the result of all signal-independent sources. These include the image-intensifier background noise, sensor dark-current noise and noise...
produced when the sensor is read (read noise). Nonuniform response in CCD and TV detectors is introduced by absorption in the windows, non-uniformities in the X-ray converter phosphor, flaws in the fiber-optic plates and tapers, the inherent properties of the image intensifier(s) and lens(es) and variations in the pixel-to-pixel response and the global response of the sensor (Deckman & Gruner, 1986; Thomas, 1990; Kalata & Golub, 1988). For multiwire proportional detectors, variations in the wire geometry lead to spatial and apparent sensitivity non-linearities; variations in X-ray path lengths, window absorption, amplifier gains and noise cause nonuniform response (Hamlin, 1985; Sobottka, Chandros, Cormick, Kretsinger & Rains, 1990; Derewenda & Helliwell, 1989). Time-dependent background changes result primarily from drifts in electronic circuits, which are often the result of temperature fluctuations. Time-dependent intensity distortions result primarily from drifts in the incident X-ray beam intensity.

As with other methods, we collect three detector calibration images: a background image, a flat-field image and a mask image. The background image is taken in the absence of X-rays. The mask and flat-field images are made by illuminating the detector with an X-ray source, with and without an X-ray-opaque metal plate containing a square array of holes (the mask). A reference flat-field image can also be recorded on an X-ray film placed at the detector position, or calculated from the known source geometry. The spatial distortions are determined by comparing the recorded mask image to the true mask geometry. The response nonuniformity is then determined by comparing the flat-field image with the reference image, after the measured spatial distortions introduced by the detector have been applied to the reference image. Once the total response has been parameterized, images can be mapped from undistorted space (detector front surface) to distorted space (pixel image output from the sensor) or vice versa.

An exact calibration correction would take into account the point-response function at every pixel (Thomas, 1990). For any real instrument, this function extends over many neighboring pixels, so that the response measured at a given pixel is correlated with events occurring at other pixels. However, it would be experimentally impractical to measure accurately the point response at every pixel. In our procedure we ignore the response correlation when analyzing the mask and flat-field images, assuming that the response at each pixel is independent of the neighboring pixels. The magnitude of the errors introduced by neglecting the effects of the extended point-response function depends on the form of the function, particularly the extent of the tails and the local pixel-to-pixel differences in sensitivity. The largest errors occur at the edges of the active image.

**Collecting calibration data**

**X-ray source**

The X-ray source can be an X-ray tube target, a radioactive isotope or a diffuse scatterer. We use a Cu-target X-ray generator to make mask, flat-field and reference images. An ideal source would be a tunable strong monochromatic point source. Radiation emitted from an X-ray generator is not monochromatic and is not necessarily uniform over the detector active area. However, if the generator is operated at the appropriate voltage and absorbers (X-ray film) are used to make the beam more monochromatic by preferentially absorbing lower-energy X-ray photons, the output beam is nearly monochromatic and relatively uniform. For example, operating at 8.4 kV with several X-ray-film absorbers gives a spectrum with > 90% of the energy between 7.6 and 8.4 kV. To calibrate our detector, we use a rotating-anode beam line with a 1 m source-to-detector distance. The detector views the source directly at a 7° take-off angle down a 10 cm diameter shielding tube. With two Kodak DEF X-ray film absorbers, the X-ray flux at the detector face is \( \sim 10^2 \) X-ray photons mm\(^{-1}\) s\(^{-1}\) with the generator operating at 8.4 kV and 1 mA, and \( \sim 10^3 \) X-ray photons mm\(^{-1}\) s\(^{-1}\) at 10.5 kV and 1 mA. We experimented with the use of metal-foil absorbers to monochromate the beam, but found that non-uniformities in the foils led to a nonuniform intensity distribution over the detector surface.

\( ^{55}\text{Fe} \) and \( ^{63}\text{Ni} \) sources are often used to calibrate area detectors, but the flux from these 0.010 to 0.050 Ci sources (1 Ci = 3.7 × 10\(^{10}\) Bq s\(^{-1}\)) is typically <10% of that from the filtered beam from an X-ray generator. \( ^{55}\text{Fe} \) decays by \( \gamma \) emission (5.9 keV, half-life 2.7 y); \( ^{63}\text{Ni} \) decays by electron emission (66 keV, half-life 96 y) and therefore forms an X-ray source when plated onto a substrate. We have used a source containing 0.015 Ci of \( ^{63}\text{Ni} \) plated onto Cu foil (a miniature Cu-target X-ray generator). This source is useful for monitoring the long-term stability of the detector, although the energy spectrum extends to 66 keV.

The use of an Fe fluorescence source (magnetic tape placed in the beam at the crystal position) has been described by Thomas (1990). This technique is difficult to implement because the scattered intensity is relatively weak and the distribution is nonuniform.

**Background images**

Background images are collected at the start of every data-collection session. Fig. 1(a) shows a typical background image. The X-ray shutter is closed and data is collected. The background-image integration time must be sufficiently long to obtain accurate statistics. To reduce the background and minimize...
variations in the background, we regulate the temperature of the image intensifiers and sensors in our detectors. For detectors with image intensifiers that are not temperature regulated, background images must be recorded more frequently during data collection.

Flat-field images

Flat-field images with \( \sim 10^5 \) X-ray photons pixel\(^{-1}\) are recorded in about 1 h using the X-ray generator operating at 8.4 kV with two to four DEF film absorbers (Fig. 1b). Flat-field images made with the 0.015 Ci \( ^{63}\)Ni source 10 cm from the detector face require 5 h to obtain \( \sim 10^4 \) X-ray photons pixel\(^{-1}\) (\( \sim 10 \) X-ray photons mm\(^{-2}\) s\(^{-1}\)). For this source, since the distribution of radioactivity and the absorption of the detector windows are known, the intensity distribution at the detector face can be calculated.

Reference images

The intensity distribution at the detector face produced by an X-ray generator is not necessarily uniform. We measure the distribution with Kodak DEF X-ray film placed at the position of the detector, exposed at the same operating voltage as used for collecting the detector flat-field image. The film is developed with intermittent N\(_2\) agitation and the optical density is digitized to 8 bits with an Optronics P-1000 film scanner (Optronics, Inc., Chelmsford, MA) and converted to equivalent intensity (Phillips & Phillips, 1985). The optical density is partitioned into

Fig. 1. Calibration images for the Bandeis SIT vidicon detector. (a) Background image, (b) flat-field image, (c) digitized reference image and (d) mask image. The background image was accumulated for the same time as the flat-field image, but the z scale here is multiplied by a factor of 20 to show detail in the noise. Flat-field and reference images were made with four Kodak DEF X-ray film absorbers in the beam, with the generator operated at 8.4 kV and 5 mA, exposure time of 30 and 150 min respectively; the mask image was made at 9.5 kV and 5 mA, exposure time of 60 min. The source-to-detector distance was 1 m; the pixel size is 0.26 mm in each image.
pixels equal in size to the pixels on the detector face (as determined by the mask-fitting routine \textit{CALPRM} discussed below) and smoothed to remove effects of dust \textit{etc.} (Fig. 1c). The local pixel-to-pixel intensity variation, measured by scanning the same film several times, is 1 least-significant bit (<\frac{1}{2}\%).

\textbf{Mask images}

The masks we use are fabricated from a 0.075 mm BeCu sheet by photo-etching a square array of holes (Max Levy Inc., Philadelphia, PA).* Two different masks have been made: a lower-resolution mask for calibrating our vidicon-based detector (Fig. 1d) and a higher-resolution mask used for calibrating our CCD-based detector (Fig. 2). The masks are plated on both sides with 0.005 mm of gold to make them effectively opaque to X-ray photons with wavelengths >1.0 Å. The higher-resolution mask has 0.150 mm diameter holes with a center-to-center separation of 1.01 mm; the lower-resolution mask has 0.635 mm diameter holes with a separation of 2.26 mm. The distance between hole centers is small enough to allow spatial distortions to be adequately sampled, large enough to keep adjacent spots separated and accurately spaced. (The 5 mm hole spacing of the mask supplied with the Siemens detector is too coarse to allow an accurate determination of the spatial distortions produced by typical fiber-optic tapers.)

\textbf{Time-dependent variations}

Intensity drifts of the incident beam for both synchrotron and laboratory sources must be measured to scale sequential images correctly. Usually the beam intensity is monitored with an ionization chamber (Arndt & Stubbings, 1988). We convert the output of an ionization chamber to pulses with a voltage-to-frequency converter. The number of monitor pulses accumulated during the acquisition of each image can be used to scale the pixel intensities in each image. Alternatively, the image-acquisition interval can be set for a fixed number of monitor pulses.

\textbf{Long-term stability}

The response of the detector must be measured from time to time to ensure that no significant change in response has occurred. When crystallographic data are not being collected, we collect flat-field images for 10 to 20 h with a $^{63}$Ni source placed at a fixed position in front of the detector. These images are compared with similar images previously recorded. Pixel-to-pixel differences between images are typically \sim 1\% over periods of many weeks.

* The calibration routines and masks are available from the authors.

\textit{Point-response function}

The point-response function is measured at several positions on the detector with a beam whose width is much smaller than the instrumental resolution (Fig. 3). The typical variation in the response to a locally uniform input signal for the vidicon detector can be seen in the flat-field image in Fig. 1(b). From the flat-field image and the point-response function, an estimate can be made of the significance of the effects of neighboring pixels on the response of a central pixel. We conclude that the effects are of the order of 1\%, except within 5 pixels of the edge of the active area. Thus in our analysis we assume that the response of each pixel is independent of all others, but for quantitative studies we do not use data collected within 5 pixels of the edge of the image.

\textit{Response saturation}

For CCD and vidicon detectors, saturation can occur when either the sensor or the A/D converter is saturated. For CCD detectors, the sensor saturates when the CCD well depth is exceeded, which is effectively independent of position. However, for a vidicon detector, the saturation varies over the active area (Kalata & Golub, 1988). To utilize the full dynamic range of the sensor, the A/D converter gain can be set such that the sensor will saturate before the A/D converter. This will not introduce any additional quantization noise if the converter digitizes to enough bits (12 bits is sufficient for our detectors). To

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{Mask image recorded in 5 min with the Brandeis CCD-based detector, with the X-ray generator operating at 7 kV and 20 mA, with three Kodak DEF film absorbers in the beam. The pixel size is 0.065 mm.}
\end{figure}
determine the saturation level at each pixel for our vidicon detector, a series of images is collected as a function of the incident intensity and the saturation response is mapped using the program FNDSA. The saturation value at each position used during data collection is this maximum intensity value multiplied by a user-determined reduction factor, which ensures that data are not allowed to reach 100% saturation.

Calculating spatial-distortion corrections

The program CALPRM determines the spatial distortions and writes to a file the information necessary to make transformations from a distorted position (detector memory) to an undistorted position (on the detector face) or vice versa. This is described in three steps: searching the mask image to locate and determine the centroid of all the mask points; modeling the radial distortion; and modeling the local distortions.

1. Find mask points. An ordered search for peaks that represent the mask holes is performed. The user specifies peak-searching parameters, which are guides for the program and do not have to be accurately specified. First a peak is found near the center, then an adjacent peak is searched for at a position suggested by the known mask geometry. The search continues by moving horizontally and vertically across the mask looking for peaks at positions predicted from the positions of peaks previously found. The search is stopped when either the edge of the detector active area is reached or peaks are not found near their predicted positions.

2. Model radial distortion. The distortion is modeled by a second-order radial function. To determine the center of distortion, a second-order polynomial is fitted to each row and each column of peaks. The coefficients from these fits are then fitted to a second-order polynomial as a function of row or column number. If there is radial distortion, the row (or column) that goes through the center of distortion is determined by the second-order coefficient intercept. The slope of the center line, which is the same as the mask angle, is determined by the value at the center of distortion of the first-order coefficients. The intercept of the center line can be found from the zeroth-order fit. The center of distortion in pixel coordinates can now be found by the intercept of the two center lines. To determine the spacing between mask rows (or columns), the intercept between each of the rows (or columns) and the center line is fitted as a function of the row (or column) number. The spacing is the slope of this curve as it goes through the center. Calculated positions for each of the observed mask points can be determined by point index, mask angle and row and column spacing. If there is radial distortion, a radial correction with an origin at the center of distortion is applied and a new position for each peak is calculated. To correct for pin-cushion radial distortion, pixels are moved inward according to the function

\[ R_c = R_o + bR_o^2 + cR_o^3 \]  

where \( R_o \) is the observed radius and \( R_c \) is the corrected radius.

3. Model local distortions. For each mask point there are now three positions that are known: the observed (distorted) position, the calculated position (undistorted) based on the mask geometry and the observed position after correction for radial distortion. The difference between the calculated mask position and the observed position corrected for radial distortion is the local distortion. The correction for local distortion to be applied to any pixel can be determined by interpolation from the surrounding mask points. We use an interpolation based on a B spline to model the data.

The position of any pixel in distorted space can now be determined from the undistorted position by...
CORRECTING DISTORTIONS IN AREA DETECTORS

applying both local and radial distortion. Interpolation tables are made specifying the transformed position for each pixel: the 'Reverse' interpolation tables specify how to move from an undistorted image to a distorted image, while the 'Forward' interpolation tables specify how to move from a distorted image to a undistorted image. To save space, only a subset of pixel positions are saved in the interpolation tables; other pixel transformations can be determined by interpolation from surrounding positions.

Fig. 4 shows a contour plot of the interpolation tables made by CALPRM for the mask in Fig. 1(d). The plot illustrates the spatial distortions introduced by the two image intensifiers and fiber-optic tapers. Calculation of the interpolation tables on a MicroVAX III takes about 4 min and, after finding the mask points, proceeds without user intervention.

Calculating nonuniform-response correction

There are two types of corrections for the variation in response over the detector area that must be applied to any detector image: a background correction and a scale-factor correction. The background correction is made by subtracting from the data image a background image made in the absence of X-rays. The scale factor describes the response of each pixel to an input signal and is determined by the combined response of each element in the signal chain.

The nonuniform-response corrections are based on the comparison of a flat-field image (with background subtracted) with a reference image of the same input recorded on film (with film fog subtracted) or are calculated. In the absence of any spatial distortions, the nonuniformity correction matrix could be determined from a pixel-to-pixel comparison of the detector and reference images of the flat field. Because the detector image is spatially distorted and the reference image is not distorted, either the spatial distortions in the detector image must be corrected or the reference image must be spatially distorted to match the detector image. The choice between these two approaches depends on how the information in images collected during experiments is to be analyzed. When the intensity measured at each pixel is significant, for example when studying diffuse scattering, it is appropriate to correct the entire image spatially and then correct for the nonuniform response. When only a small fraction of the image is to be analyzed, for example in measuring the Bragg peaks in crystallographic studies, it is not necessary to correct the full image. Rather, the nonuniform-response corrections can be made on the spatially distorted image in the regions occupied by the peaks.

In the example in the next section we distort the reference image; we could just as well have corrected the distortions in the flat field.

Transform a reference image

The algorithm MODELFLAT has been developed to apply spatial distortions to reference images and flat fields. This algorithm, which is accurate only for images with slowly varying intensity, will apply spatial distortions without introducing artificial local intensity fluctuations, but it does not rigorously account for all of the intensity. This is not a limitation when operating on flat-field or reference images, but MODELFLAT would introduce intensity distortions in an image containing significant structure, e.g. a diffraction pattern.

To make a distorted reference image, MODELFLAT performs the following steps for each pixel in the distorted image that is being created.

1. Calculate the position of the center and the edges of this pixel projected onto the undistorted image.
2. Calculate the area of the projected pixel in the undistorted image from the positions of the projection of the edges.
3. Assign to this pixel a value equal to the value of the pixel in the undistorted image that is closest to the projection of the center, multiplied by the area of the projected pixel.

Calculate nonuniform-response correction matrix

The nonuniformity correction matrix is an array containing the ratio of the reference flat-field value to the observed flat-field value, with all invalid pixels identified.
Since the flat-field and background images should be smoothly varying, a search is performed to identify and mark all bad pixels. These pixels are identified by user-selectable criteria: the amount a given pixel differs from the average of the surrounding pixels, minimum and maximum valid pixel intensities and the limits of the detector active area. Bad pixels are typically caused by flaws in the sensor, phosphor converter and fiber-optics. The spatially distorted reference image is then divided by an image created by the subtraction of the background image from the observed flat field and the result is the nonuniformity correction matrix. Any pixels flagged as bad in either the background or flat-field images are also flagged in the correction matrix. Most bad pixels are located at the edge of the active area. If the active area is smaller than the detector image that is read out, pixels outside the active area are marked as bad. To save space, the matrix is multiplied by a scale factor and written to a file as a 2 byte (16 bit) integer array. These functions are performed by the program \texttt{MAKENON-UNF}.

Distorted reference images are extremely sensitive to spatial distortions. Incorrect modeling of spatial distortions can cause large errors in the nonuniformity correction matrix, because the matrix is based on relative pixel size. If the distortion parameters have been well determined, nonuniformities in the distorted image are the result of real local spatial distortions. However, if the distortion parameters are not well determined, either as a result of an inaccurate mask or from a poor detector image of the mask, these nonuniformities could be the result of measurement artifacts. When the mask points are not accurately determined use of a correction based only on the radial distortion produces a more accurate nonuniform-response correction matrix since the radial distortion is a function of the average of the mask points.

**Applying distortion corrections**

The distortion corrections can be applied to an entire image or to just a portion of the image. For most X-ray crystallographic applications, only a portion of the image (that of the Bragg peaks) is of interest. In this case, only the region surrounding the Bragg peaks is corrected. For other applications, such as studying diffuse scatter, the entire image must be corrected.

Two algorithms have been developed to apply spatial distortions to images: \texttt{MODELFLAT} (described in the previous section), which is appropriate

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Fig. 5. (a) Image of a mask (with background subtracted) taken with the vidicon-based detector system; holes are 0.64 mm in diameter and spaced 2.26 mm apart. (b) Mask image after correction for nonuniform response. (c) Mask image after correction for nonuniform response and spatial distortion. The lower plots are traces through one row of spots. In (c), variations in the heights of adjacent peaks are due to counting statistics; the fall-off in height and increase in width of peaks near the edges of the image are due to defocusing in the image intensifiers.
for images in which the intensity varies slowly from pixel to pixel (e.g. reference images) and **INTERPOLATE**, which is appropriate for crystal diffraction patterns and mask images.

**Applying corrections to entire images**

Applying the corrections to entire images is performed in three sequential steps: subtract background, correct nonuniformity and correct spatial distortions. This is demonstrated in Fig. 5

1. **Subtract background.** The background image is first subtracted from the raw data image (Fig. 5a). If the integration times are not the same, the background image is scaled to the data image. On our (and most other) detectors, there is an area in each corner of the image where only background accumulates. We use this region to scale the background and data images.

2. **Apply nonuniform-response correction.** For each pixel position, the intensity value is multiplied by the corresponding value in the nonuniformity correction matrix, divided by the average nonuniformity correction value near the center of the image. If the correction matrix contains a bad-pixel flag, this position can also be flagged as bad. This correction is applied to entire images by the program **NORMALIZE**.

3. **Apply correction for spatial distortion.** The program **INTERPOLATE** either corrects for or applies the spatial distortions in an entire image. Input includes the interpolation tables created by **CALPRM** and the image to be transformed. For a given pixel in the image, the transformed position of the center of each edge is calculated. Through these four points a rectangular box is drawn in the transformed image. The intensity in the original pixel is then divided between all the pixels in the transformed image that fall under this box by an amount proportional to the overlap (Fig. 6). The intensity (ADU units) of each pixel is preserved and the total intensity in each image is the same. This algorithm, which is a compromise between speed and accuracy, would work correctly if the edges of the transformed box were truly straight lines. Since the edges are, in general, curved, the algorithm produces small errors because a fraction of the intensity is shifted incorrectly to an adjacent pixel, as shown in Fig. 6. For crystallographic data this error is of no consequence because all intensity is conserved.

There are alternate computational approaches that conserve intensity and minimize these errors. The most common approach is to calculate the transformation on a smaller scale to approximate the curved edges of the transformed pixel more closely. To do this, the intensity from each pixel is redistributed to a set of identical subpixels, each of which is transformed individually. As the size of the subpixel decreases, the error in the transformation becomes smaller, while the time to perform the transformation increases as the number of subpixels. We found each pixel had to be divided into 1000 subpixels to decrease the error in the transformation significantly. Another approach is to approximate the transformation by a set of quadrilaterals instead of rectangles. This method also produces (smaller) binning errors but it is computationally more difficult and more CPU intensive. Fig. 5(c) shows the results of **INTERPOLATE** operating on an image of the mask. On a MicroVAX III this program takes approximately 30 s to calculate a transformed image. There are no apparent spatial distortions introduced by this method.

**Applying distortion corrections to small regions of the image during data collection**

The **MADNES** X-ray crystallographic data-collection package (Messerschmidt & Pflugrath, 1987) was modified to utilize these distortion corrections. During data collection, the image is not corrected for spatial distortion. Instead, the predicted position of a Bragg peak in mm relative to the beam is converted to a pixel position in the distorted image using the interpolation tables created by **CALPRM**. Then only the region around that distorted position is corrected for the intensity distortions. These corrections include: background subtraction, scaling by the nonuniform-response correction, scaling by the time-dependent correction and checking for saturation. The time-dependent scale factor is determined from the ratio of the number of monitor counts in the current image divided by the average number of monitor counts. If the correction matrix contains a bad-pixel flag, this position can also be flagged as bad. These routines were used with the Brandeis vidicon, Brandeis CCD, Argonne CCD and Siemens multiwire detector.

![Fig. 6](image.png)
systems. The functions of MADNES that require accurate spatial distortion corrections are auto-indexing, refinement and the prediction of peak positions during data collection. With all four detector systems, these functions proceeded without problems.

**Evaluation of distortion corrections**

**Nonuniform response**

For the vidicon detector, many flat-field images were collected over a period of weeks. After correction using the same nonuniformity correction matrix values, these images scaled to approximately 1% at each pixel, as long as the temperature of the detector was constant to ~0.2 K.

To demonstrate that a correction method based on data from flat-field images can correct X-ray crystallographic data, the accuracy of the correction was evaluated by measuring the intensity of the (200) Bragg reflection from a stationary LiF crystal at many positions on the detector surface. After background correction, nonuniformity correction and beam-monitor scaling of the images, the standard deviation of the distribution of observed peak intensities was equal to the standard deviation expected from the counting statistics (2%).

**Spatial distortions**

Because of the B-spline interpolations, if the distortion corrections calculated from a mask image are applied to the same mask image, an essentially perfect correction should result. To test the accuracy of the correction, the correction should be applied to an image in which the peak positions are known but are different from those in the original mask. The transformed peak positions can then be compared to the known positions. To perform this test, a correction matrix was first generated from a mask image made with the vidicon detector. Then the mask was translated and rotated, moving the mask holes to different (known) image positions and a second mask image was recorded. While the overall geometry of the second image is similar to that of the first, on a pixel scale the images are entirely different and therefore serve as a test of the method. The standard deviation of the distribution of the differences between the corrected and the known positions was <0.1 pixel.

**Discussion**

Routines have been written to determine the spatial distortions produced by optical and electro-optical components of detector systems, correct images for spatial distortions, model the intensity transformation produced by the spatial distortion corrections and correct for nonuniform intensity response. These routines make approximate corrections for spatial distortions and nonuniform response, as is true for other empirical correction procedures that have been developed. Unlike other methods (Durbin, Burns, Mulai, Metcalf, Harrison & Wiley, 1986; Kabsch, 1988; Thomas, 1989), our method models spatial distortions with a radial function and an interpolation table, which correspond to the geometrical distortions present in many detectors. Our method can either correct for, or apply, spatial distortions. We are generally interested in crystallographic data where Bragg-peak intensities are being measured. In this case, it is more efficient to make the corrections to the distorted image in the area occupied by the peaks than to transform the entire data image to an undistorted image.

Apparent nonuniform response in a raw detector image results from spatial distortions as well as from the actual nonuniform response of the detector system. Because of the sensitivity of the nonuniform corrections to the spatial-distortion correction, it is important to start with an accurate map of the spatial distortions.

On the four detectors for which we have used the routines, the spatial-distortion correction is good to within 0.1 pixels, which is satisfactory for any X-ray crystallographic experiment. When these spatial-distortion corrections are used within the MADNES data-collection package, r.m.s. deviations between the predicted and observed pixel positions are consistent with the distortion-correction accuracy of 0.1 pixels. The accuracy of the nonuniform response correction with both flat-field images and Bragg peaks is ~2%.

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CORRECTING DISTORTIONS IN AREA DETECTORS