Quality assessment system for curved crystal X-ray optics

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Doubly curved crystal X-ray optics provide intense focused monochromatic beams from laboratory X-ray tube sources. These optics are employed in crystallography and X-ray fluorescence systems and may find application to imaging. It is increasingly important to understand how optic defects impact performance for these systems. A simulation model was developed to assess the effects of misalignment and optic defects on system parameters such as intensity, beam size and resolution. Simulation results were compared to optics measurements. Rapid reproducible measurements of optics quality are important both for performing systematic studies of optics defects and for assessing individual optics. A simple operator-independent alignment technique was developed that was also beneficial in ensuring optimal beam intensity in analysis systems. The measurements and simulations were in good agreement and provided insight into essential optics parameters.

1. Introduction

Since doubly curved crystal (DCC) optics collect and focus X rays emitted into a large solid angle by a laboratory point source, they provide an increase in intensity compared to the use of flat monochromators [1,2]. They have increasingly become an established tool for X-ray applications [3], particularly in X-ray fluorescence [4,5].

A photograph of a DCC optic is shown in Fig. 1. The optic is designed so that all rays originating from the point source hit the optic at a Bragg angle, \( \theta_B \), and are diffracted towards the image point [6], as shown in Fig. 2. Because diffraction at a particular Bragg angle selects a narrow range of energies from an incident white beam, the resulting focussed beam is monochromatic. The doubly curved crystal optic is produced by pressing a thin silicon single crystal wafer between a curved substrate and a mold [7–9]. For X-ray fluorescence, the focused monochromatic excitation yields low background with high intensity for sensitive measurements in medical and material sciences and in manufacturing [10,11]. Several studies have concentrated on improving optic properties for these applications [12–14]. Monochromatic beams also have potential application in medical imaging [15,16].

The DCC optics used in this work were designed for the K\( \alpha_1 \) energy (17.478 keV) of the molybdenum X-ray source with the parameters listed in Table 1. While ideal optic performance depends on geometrical aberrations and strain [17–19], and thus is determined by the size, thickness and bending radii, real optic performance is degraded by profile error and by errors during manufacturing of the placement of the crystal segments, which creates a defect similar to mosaicity. Both manufacturing defects broaden the rocking curve and reduce the efficiency of the optic. Measurements and simulations were performed to assess these effects.

2. Simulation analysis and crystal bandwidth

A simulation was developed to model optic performance, assess optic defects, facilitate alignment trouble-shooting and model optical applications. The simulation is based on simple ray tracing, similar to that used in Shadow [20–26]. A sketch of a symmetric DCC optic using Johann geometry [6] is shown in Fig. 3.

In the simulation, the finite source is modeled by moving an ideal source over a grid of points within a finite radius of the source center. The source center itself can be moved to model source displacement. Photons are emitted from the grid point in triplets, two
Fig. 1. X-ray Optical Systems, Inc. DCC optic #A275. Ideally, all rays originating from the source point S hit the optic at the Bragg angle, \( \theta_B \), and are diffracted towards the image point I. This optic has five crystal segments; the tested optics had one and three segments. Optics used in commercial XRF systems often have a larger number of segments.

Fig. 2. Geometry of diffraction for toroidal crystals. The crystal surface is at the correct angle for diffraction at a Bragg angle \( \theta \) over its whole surface. The dashed lines represent rays which are out of the plane of the Rowland circle.

The coordinate system is then rotated to reflect possible misalignment of the optic by an in-plane angle \( \gamma \) and out-of-plane angle \( \phi \). The location of the crystal location \( \mathbf{y}_A \), calculated using X-ray Optics utilities (XOP) [25] to be approximately 60%. To assess the quality of the optic, the experimentally determined rocking curve width was compared to the theoretical value. The theoretical crystal bandwidth due to in-plane bending can be estimated using the geometry shown in Fig. 4. Because of the oblique incidence, the ray hits planes on the exit side of the crystal at a different angle than planes at the surface [17,28].

The resulting broadening is

\[
\Delta \theta_b = \delta \approx \frac{T}{2R \tan \theta_B},
\]

where \( \theta_B \) is the Bragg angle at the particular K\( \alpha \) line. To determine absolute intensity, the probability of diffraction was multiplied by the average peak reflectivity for the curved silicon, calculated using X-ray Optics utilities (XOP) [25] to be approximately 60%. To assess the quality of the optic, the experimentally determined rocking curve width was compared to the theoretical value.

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### Table 1

<table>
<thead>
<tr>
<th>Optic</th>
<th>Input/output focal distance (mm)</th>
<th>Optic size (mm²)</th>
<th>Input angular width</th>
<th>In-plane bending radius (mm)</th>
<th>Out-of-plane bending radius (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>115A</td>
<td>120</td>
<td>7 × 17.4</td>
<td>0.6° × 8.4°</td>
<td>650</td>
<td>22</td>
</tr>
<tr>
<td>A723</td>
<td>193</td>
<td>11.5 × 45</td>
<td>0.6° × 13.4°</td>
<td>1030</td>
<td>35</td>
</tr>
</tbody>
</table>
resulting change in d spacing gives a change in Bragg angle, so that
the broadening in crystal bandwidth due to the out-of-plane bend-
ing is \[ |\Delta \theta_B| = \frac{T}{r} \tan \theta_B. \] \( \tag{8} \)

The Poisson ratio for silicon is approximately 0.28 \([30]\), so there is an additional 0.003° of bandwidth due to the out-of-plane bend-
ing. The theoretical bandwidth for an ideal optic with a focal length of 190 mm and a thickness of 40 μm is thus approximately 0.015°.

Given the crystal bandwidth and the incident angle, a random number generator is used in the simulation with the probability given in Eq. (5) to determine whether the ray diffracts. Once the ray has been diffracted from the crystal surface, it changes direction to \[ \text{ray}_{\text{after}} = \text{ray} - 2\hat{h}(\text{ray} \cdot \hat{h}), \] \( \tag{9} \)
and propagates towards the image plane.

3. Experimental set-up

In order to obtain reproducible measurements for optics assessment, and to obtain maximum intensity from the optics, the alignment must be precisely optimized in six degrees of freedom. In practice, because displacement in one axis shifts the intensity peak in other axes away from the proper aligned value, misalignment in one axis propagates to other axes. It can be difficult and time consuming to insure optimal performance, since maximizing a single variable at a time will not necessarily produce the optimal position. A simple, rapid, reproducible alignment technique has been developed in this study. The simulation was used to verify that the ordering of the steps mitigates the propagation of misalignment.

3.1. Source alignment

A laser was used to establish a beam path, and to allow for rough pre-alignment of the source and optic. Using a laser system decreases the alignment time and increases repeatability. An arbitrary beam path was first established by placing a laser at a fixed height and angle to the optical table. Alignment to a predetermined path is required for most medical imaging applications, as well as many commercial X-ray diffraction (XRD) and X-ray fluorescence (XRF) systems. The source was then aligned to the laser by first aligning a rail to the laser and then aligning the source to the rail. Depending on system constraints, these steps could be reordered.
For example, the laser could be aligned to a fixed rail and, for a fixed source, the rail could be first aligned to the source.

To aid the first step for this measurement system, alignment of the rail to the laser, two washers were placed separately on carriers on an optical rail. The washers then were adjusted so that the laser passed through their centers, as shown in Fig. 6. The diameter of the hole in the washers was 3 mm, about three times the diameter of the laser beam, so that alignment of the laser beam had an accuracy better than 0.5 mm. The rail was aligned parallel to the laser by translating, tilting and rotating the rail until the washers stayed aligned as the rail carriers were moved along its length. Alternatively, for a fixed rail system, it is the laser which must be translated, rotated and tilted until the beam is parallel to the rail and the washers remain aligned when translated.

The X-ray source was an Oxford Ultra-Bright with a molybdenum anode. Alignment was typically performed at low power, 24 kV and 0.5 mA, to diminish source aging. Application measurements were made up to 40 kV and 1 mA. Previous measurements of source size and location show minimal change over this range of powers [31]. The source diameter was measured to be 100 ± 10 μm using pinhole images at a series of source distances [32,33]. That gives a source divergence (source radius/source-to-optic distance) of 0.015°, similar to the theoretical bandwidth of the optic. Sources with larger diameters would not be as efficiently utilized because X rays emerging from the edges of the source would hit the optic center at an angle larger than the angular acceptance width of the optic.

The source was mounted on the rail. The laser was protected with a lead shield during X-ray exposure. The source position was adjusted to the rail by observing its position on a camera system consisting of an image intensifying screen with a low cost CCD imager. Images could be recorded using Zio Corporation Camera Mate video software, although with poor resolution and linearity. Images suitable for data analysis were recorded with a Fuji restimuable phosphor plate system, as shown in Fig. 7(a).

The combination of shadowing from the X-ray anode and window aperture within the X-ray tube produced a beam of radiation from the source which was narrow in the horizontal direction, as seen in Fig. 7(a). It was necessary to translate the source until the most intense part of the radiation beam passed through the center of the first washer. After alignment of the beam with the rail, the most intense part of the beam was placed where it will intercept the optic. To align the X-ray beam from the source with the rail, the source was rotated until the shadows of two washers were concentric, as shown in Fig. 7(b). As the rotation axis did not pass through the source anode, it was necessary to shift the source position after each rotation to maintain the alignment of Fig. 7(a).

For a fixed source, the rail could be aligned to the source by translating and rotating the rail until the images shown in Fig. 7 are achieved, and then aligning the laser to the rail.

3.2. Measurement system

Fig. 8 shows the experimental setup, with six degrees of freedom: translation parallel to the rail (z axis), and in the horizontal (x) and vertical (y) directions perpendicular to rail; rotation about the vertical axis; and tilt about the two horizontal axes. Except for the two axis manual tilt stage, all the axes were adjustable under computer control. Because motion along the z direction beyond the range of the motorized stages was needed to measure the optic performance as a function of source-to-optic distance, the whole optic setup was mounted on the optical rail.

4. Optic rough alignment

A five step alignment procedure was developed to ensure accurate positioning of the optic. To allow for rough visual alignment of the optic, a second laser was placed collinear with the first, but pointing away from the source, as shown in Fig. 9. The second laser was placed on a rail carrier, which allowed for reproducible repositioning after removal from the X-ray beam. Before the X-ray
source was turned on, laser 2, on its rail carrier, was first removed from the rail so that it would not shadow the X-ray beam before it intercepted the optic. When laser 2 was replaced on the rail for use in aligning the optic, the optic was first translated out of the way under computer control and the alignment of laser 2 with laser 1 was verified. Laser 1 was then not used except to verify the alignment of the laser 2.

4.1. Center optic on rotation axis

If the center of the optic is not over the center of the rotation axis, then the X-ray beam shifts relative to the optic center when the optic is rotated. To avoid this, the motion of the beam spot from laser 2 was observed on the crystal as the crystal was rotated, as shown in Fig. 10. The placement of the optic on the rotation stage was corrected until the beam spot remained stationary.

4.2. Center optic horizontally

The optic was then rotated to face the laser 2. The optic was moved horizontally (along the x axis) until the laser hit the left and right edges of the optic, reading the length of travel between them, and moved half-way between to be centered horizontally. The optic was not moved again in the x direction during the experiment because that would move the optic center away from the most intense part of the X-ray beam as seen in Fig. 7(a).

4.3. Step 3: center optic vertically and adjust horizontal tilt

The optic was translated vertically until the laser beam hit the upper and then the lower edge of the optic, and then centered. While the optic was being translated vertically, it was observed whether the laser spot remained centered horizontally. If the optic is tilted about the z axis, then the laser spot shifts horizontally across the optic face as the optic is moved vertically, as shown in the diagram in Fig. 11. This was corrected by manually adjusting the tilt stage to rotate the optic about the laser beam axis.

4.4. Step 4: align rotation and vertical tilt

Because the optic is curved, if the optic is not centered vertically, the back reflected laser beam will hit the laser above or below the incident beam. However, even if the laser is centered vertically, the back reflected beam can still be reflected up or down if the optic is tilted towards the laser, as shown in Fig. 12. The tilt screw was manually adjusted until the reflected beam was at the same height as the incident beam when the optic was centered vertically. The optic rotation was adjusted so that the back reflected laser spot was coincident horizontally with the incident beam. Finally, the optic was rotated by $90 - \theta_B$, where $\theta_B$ is the Bragg angle, as shown in Fig. 13. Lead shielding was later added after the optic to block the direct beam, as shown in Fig. 13.

4.5. Step 5: rough determination of input and output focal distance with CCD camera

The optic is now at the right orientation to the X-ray beam, but not necessarily at the correct distance from the source. The CCD

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Fig. 9. Experimental set-up with the second laser added collinear to the first.

Fig. 10. Top view of the set-up of the DCC optic. If the center of rotation is in front of the optic, as shown at top, the laser spot moves relative to the optic center in the direction opposite to the rotation. If the center of rotation is beyond the optic, as shown in the bottom diagram, the laser spot moves in the direction of rotation.

Fig. 11. If the optic face is tilted, vertical motion causes a sideways shift of the laser beam spot with respect to the optic face. The tilt screw was used to adjust the optic so that the spot remained centered horizontally as the optic was shifted vertically.

Fig. 12. Side view of set-up. When the optic was tilted, the back reflected laser beam hit above or below the incident beam.
Author’s personal copy

camera system was used to roughly determine the output focal distance. The camera was mounted on horizontal computer controlled stages and initially placed near the optic in the path of the reflected laser beam, as shown in Fig. 13. The diffracted output image was observed while rotating the optic slightly to maximize the intensity. The effect of rotation on the output image is shown in Fig. 14. The optic was then adjusted vertically to maximize the area of the optic arc in Fig. 14(a). The image shows that nearly the entire height and width of the optic is illuminated. Optic rotation to maximize intensity was repeated after each vertical move. After maximizing the image size and brightness, the camera was then moved away from the optic to find the output focal point, where the beam size is smallest. The approximate focal distance between the optic and the camera was recorded. For a symmetric optic, the output focal distance should be approximately the same as the input focal distance.

5. Optic fine alignment and assessment

5.1. Input focal length

Simply observing a bright spot on the camera is not adequate to verify optic alignment. As expected from the geometry of Fig. 3 (and demonstrated in Section 5.3) the location of the apparent output focal spot changes with the source-to-optic distance. Thus quantitative information is required to accomplish the final alignment of the optic. A Canberra high purity germanium (HPGe) detector was placed near the output focal point of the optic. About 3.2 mm of aluminum was used on the detector to prevent detector saturation. The diffracted spectrum from the optic shown in Fig. 15 shows the Kα peak without Kβ and bremsstrahlung, which is an indication that the source, optic and detector are well aligned.

With the detector aligned, the intensity was recorded as a function of optic rotation, as shown in Fig. 16. For all the measured data, a constant offset due to air scatter and scattering from the crystal was subtracted before normalization. The normalized rotation scan data were then fitted with a Gaussian (not shown), used to estimate peak width. The distance, z, between the source and the optic was changed and the rotation scan was repeated. The input focal distance is the distance at which the rotation scan width is a minimum, 192 ± 3 mm for optic A723, as shown in Fig. 17. The minimum width of the rotation scan for optic 115A, as shown in Fig. 14. (a) CCD camera image of aligned optic #115A, and (b) simulated image. (c) Image and (d) simulation of optic rotated by Δθ = 0.6°. Images were taken at 28 kV and 28 W, with the camera 55 mm from the optic. The image size is approximately 30 mm x 8 mm.

Fig. 13. Top view of the set-up after rotating the optic to the Bragg angle θB. The lead shield was used to block the direct X-ray beam.

Fig. 14. (a) CCD camera image of aligned optic #115A, and (b) simulated image. (c) Image and (d) simulation of optic rotated by Δθ = 0.6°. Images were taken at 28 kV and 28 W, with the camera 55 mm from the optic. The image size is approximately 30 mm x 8 mm.

Fig. 15. Output spectrum of DCC optic A723. The width of the peak (FWHM = 0.3 keV) is due to the energy resolution of the HPGe detector.

Fig. 16. Output intensity versus rotation angle for optic A723. A slight shoulder in the data and simulation near 0.06° is due to the Kα2 line. The crystal bandwidth was varied as a fitting parameter in the simulation, as discussed in Section 5.2. A value of 0.05° gave the best fit.

Fig. 17. Width of the rotation scan versus optic-to-source distance for optic A723. The input focal distance is at the minimum, 192 ± 3 mm.
Fig. 18, occurred at 121 ± 4 mm, which is also the location of maximum intensity, as shown in Fig. 19.

5.2. Crystal bandwidth

Once the input focal point had been determined, the measured rotation scan at the focal point was compared to the simulated scan computed with different values of the crystal bandwidth, as shown in Fig. 16. To obtain the best fit, the required crystal bandwidth for optic A723 was 0.050 ± 0.005°, a factor of three higher than the theoretical crystal bandwidth. A possible explanation is a manufacturing defect which has created incorrect angular displacement between the three crystal segments shown in Fig. 20. This is supported by powder diffraction data taken with this optic, which shows significant resolution degradation if multiple optic segments are illuminated [33,34].

Optic 115A had a visible defect on the surface, shown in Fig. 21. That caused a double peak in the output focal spot, as shown in Fig. 22. The crystal bandwidth required in the simulation to match the data for this optic was very large, 0.51°, as shown in Fig. 23, compared to a theoretical value of 0.024°. However, fine structure was seen in the rotation scan when the step size was decreased, also shown in Fig. 23. The second data set is a good fit to the normalized sum of the original simulation and a second simulation using the theoretical bandwidth. Both data and simulation resolve the Kα doublet, which has a separation of 0.065°. This is consistent with a mosaic structure in the optic itself, i.e. areas of nearly perfect optic at slight angles to each other due to the visible defect.
5.3. Simulated source-optic alignment scans

The crystal bandwidth in the simulation was then set to the empirically determined values, 0.05 /C176 for optic A723 and 0.51 /C176 for optic 115A. The resulting agreement between the simulated and measured input focal distance is good, as shown in Figs. 18 and 19. The simulation allows analysis of the often seen effect that displacement in one of the six axes affects the others. For example, if the source is deliberately displaced in z, i.e. if the source-to-optic distance is decreased, not only is the width of the rotation scan increased, as was seen in Figs. 17 and 18, but the peak is displaced, as shown Fig. 24. Tilt displacement also broadens rotational scans, as shown in Fig. 25. The simulation allows systematic assessment of the effects of multiple axis displacement. The peak broadening and shifts in peaks due to displacement in another axis demonstrate the utility of a laser system to pre-align the optic before refining the position using X-ray data.

5.4. Output focal distance and spot size

The output focal distance was determined by finding the distance from the optic at which the output spot was a minimum size. Images were taken using a Fuji restimuable phosphor image plate. A thick filter was placed in front of the source to avoid overexposing the image. An image and a profile of intensity along a horizontal cut through the image are shown in Fig. 26. This was fit to a Gaussian to determine the FWHM. A plot of the width versus optic-to-plate distance is shown in Fig. 27. The minimum of this plot corresponds to the output focal distance, which was 195 ± 3 mm for the optic A723.

### Equation (10)

\[
\text{width} = s + f(\Delta d) + g,
\]

where s is the source diameter, f is the output focal length, \(\Delta d\) is the crystal bandwidth, and g is a geometric aberration due the fact that...
the outer edge of optic toroid of radius 2R in Fig. 3 deviates from the Rowland circle [14]. The aberration g is very small, about 8 μm, for a point source, and is also small for a finite source if the optic width and height are small. However, the aberration found from a finite source in combination with a finite optic size, as given by Eqs. (1)–(9), can be significant. The ideal theoretical width from the first two terms in Eq. (10) for optic A723 is 266 μm when Δθ is the empirical crystal bandwidth of 0.05°.

The measured and simulated focal spot of Fig. 27, with the source aligned at the input focal point, is shown in Fig. 29. The simulated output image at the focal point was not an ellipse, but an X with a very narrow waist. To compare the “width” of the X to the experimental width, the standard variance was used. First the centroid values \( x \) and \( y \) were computed as

\[
x = \frac{1}{N_x N_y} \sum_{j=1}^{N_y} \sum_{k=1}^{N_x} j \delta_{j,k},
\]

\[
y = \frac{1}{N_x N_y} \sum_{j=1}^{N_y} \sum_{k=1}^{N_x} k \delta_{j,k},
\]

where \( N_x \) and \( N_y \) are the number of rows and columns, and \( j, k \) is the intensity of the \( (j,k) \)th pixel. Then the variance was taken as, e.g.

\[
\sigma_x = \sqrt{\frac{\sum_{j=1}^{N_y} \sum_{k=1}^{N_x} (x - \bar{x})^2}{N_x N_y}}.
\]

in the usual fashion. The FWHM was taken as \( 2\sigma \sqrt{2\ln(2)} \), which would be correct for a Gaussian distribution. The FWHM of the measured output focal spot for optic A723 was 274 μm × 335 μm. The simulated focal spot size was 340 μm × 380 μm, approximately 15% larger than the measured value. The simulation gave an aberration, an increase compared to the ideal theoretical value, of 70–110 μm due to the finite source and optic sizes. The simulated size continues to be in good agreement as the simulated detector is moved away from the focal point, as shown in Fig. 27.

The simulated value for the shorter focal length optic, 115A, was 109 μm × 190 μm. The ideal theoretical value, using the theoretical bandwidth of 0.024°, is 150 μm. The measured value, including the double peak, was 172 μm × 244 μm.

5.5. Efficiency of DCC optic

The efficiency of the DCC optic was taken as the ratio of the number of photons that were diffracted from the optic to the number that were incident on the face, in a 1 keV energy window around the Ka line. The count rate with the optic, \( C_w \), was measured with the HPGe detector at the output focal point. The count rate is related to the diffraction efficiency, \( \eta \), by

\[
C_w = \frac{A_{\text{optic}}}{4\pi} PT_1 \eta,
\]

where \( P \) is the source power, \( T_1 \) is the transmission of the filter used to prevent detector saturation, and \( A_{\text{optic}} \) is the optic area presented to be the beam, \( A_{\text{optic}} = HW \sin \theta_b \), where \( H \) is the optic height and \( W \) is its width.

The source power was found by recording the counts without the optic, \( C_{w/0} \), as shown in Fig. 30. The same filter, source voltage and current were used for both measurements. The count rate without the optic is given by

\[
C_{w/0} = \frac{A_{\text{aper}}}{4\pi} PT_1 \eta.
\]

where \( A_{\text{aper}} \) is the aperture area and \( L \) is the source-to-aperture distance. Thus, the diffraction efficiency was

\[
\eta = \frac{C_w}{C_{w/0}} \frac{L^2}{L^2} A_{\text{aper}}.
\]

The theoretical efficiency varies with the ratio of crystal bandwidth to source divergence. For the simulation for optic A723, using a source size of 0.1 mm, and the empirical bandwidth, which include effects of manufacturing defects which create inaccuracies in angular displacements of the crystal segments, the efficiency of was 43%. Using the theoretical bandwidth, the efficiency was 25%. Simply using the rocking curve width to fit the crystal bandwidth in the simulation does not accurately reproduce the efficiency of a defected, mosaic, optic. Each nearly perfect region can have no better efficiency than a crystal with the theoretical bandwidth. The overall efficiency is then significantly reduced because the entire optic face cannot be simultaneously aligned if manufacturing defects have created incorrect angular displacements between regions. Future work includes modifying the simulation to model mosaicity. The measured efficiency of the optic was 2% for both optics. The low measured efficiency is consistent with profile error and manufacturing defects which create incorrect angular displacements between the crystal segments. Optics of similar design have been measured by the manufacturer to have efficiencies of 16–20%.

Optic 115A and A723 were also used for early measurements before the DCC optics alignment technique was developed. The optics produced between 15% and 20% more flux when they were aligned based on the DCC optics alignment technique.

6. Conclusion

A doubly curved crystal X-ray optic alignment system was demonstrated to yield reproducible alignment of the multiple axis system to assess optics defects and to optimize performance. Two DCC optics have been tested based on this procedure. A simple optics simulation code was developed to provide understanding of the optic output, the sensitivity of the alignment parameters and optic defects. The measured crystal bandwidths were much wider than the theoretical bandwidths. This was due to manufacturing defects that result in incorrect angular relationships between different areas of the optic face, and to other crystal profile errors. The experimental results were compared with the simulations using the measured bandwidth. The simulations effectively modeled the behavior of the curved crystal optics with displacement by the six rotational and translational axes, which allows for assessment of system performance in a variety of applications.
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