Crystal tilt error and its correction in diffraction enhanced imaging system

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Abstract

In the experimental setup for Diffraction Enhanced Imaging (DEI) and its extension, Multiple-Image Radiography (MIR), it is essential to have the two or three crystals angularly aligned relative to one another around two orthogonal axes; the angle around an axis perpendicular to the diffraction plane (the Bragg angle) and also around a perpendicular axis in the plane (azimuthal angle). The appearance of the azimuthal angle (tilt error) will complicate the interpretation of the DEI/MIR images by creating a systematic change in the Bragg angle across the width of the imaging beam which in turn creates intensity variations across the imaging field. In this paper we present the effect of a tilt error, its estimation from the resulting images, and a method to correct such an error for the DEI/MIR images. The analysis and results will also apply to multiple crystal systems with tilt errors, such as monochromators on synchrotron beamlines.

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1. Introduction

Diffraction Enhanced Imaging (DEI) \cite{1} is a phase sensitive X-ray imaging method to measure an object’s X-ray transmission based on a highly collimated imaging beam which is prepared by a perfect crystal monochromator at the synchrotron facility. DEI and its extension, Multiple-Image Radiography (MIR) \cite{2,3} have shown great potential in conveying information about subtle density and structural differences in soft tissues. Many morphological features in soft tissues that are difficult or impossible to see in clinical radiography can be detected using DEI and MIR \cite{4–6}.

The experimental setup of DEI and MIR is shown in Fig. 1. This experimental setup is also commonly referred to as Analyzer Based Imaging (ABI) \cite{7}. In this article we will refer to the imaging system as a DEI system. In the commonly used DEI system, there are three crystals that have the same type of diffraction plane and all of them are set at their Bragg angle; the first two as a monochromator, the third one as an analyzer. The crystal analyzer is positioned between the object and the detector. The angle of the analyzer can be changed relative to the monochromator crystals. The angular yield function of the analyzer is described by rocking curve shown in Fig. 2. The rocking curve describes how the reflectivity of the analyzer responds to small variations, of the order of microradians (\( \mu \text{r} \)), in the directionality of the transmitted beam through

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an object. It transfers these small variations in the
directionality of the transmitted beam into large intensity
changes which results in image contrast. For example, a
direction change of 0.1 μr at 40 keV using a Si(3,3,3) crystal
set results in an approximate intensity change of 7%. This
contrast conveys the refraction and extinction or ultra
small angle X-ray scattering information of the object.

Obviously, the angular sensitivity of the DEI system
depends on the angular width of the analyzer’s rocking
curve and the position on the rocking curve to which
the analyzer is tuned. As shown in Fig. 2, the angular width
of the rocking curve further depends on the beam energy
(Fig. 2(a)) and the type of the diffraction plane of the
crystal (Fig. 2(b)). The angular sensitivity of the DEI
method can be as good as 0.01 μr [1].

The interpretation of DEI and MIR images is made by a
comparison between the rocking curves measured with
object and the intrinsic rocking curve which is acquired in
an area where no structured object is present [1–3].

\[ \lambda = 2d_{hkl} \sin \theta \]  

(1)

where \( \lambda \) is the wavelength of the incident beam, \( \theta \) is the
incident angle on the lattice planes of the crystal, and \( d_{hkl} \) is
the d-spacing of the crystal.

The incident angle \( \theta \) can be obtained by the inner
product of the reciprocal lattice vector \( \vec{G} \) of the crystal,
\( |\vec{G}| = 1/d_{hkl} \), and the incident wave vector \( \vec{k} \), \(|\vec{k}| = 1/\lambda \).

\[ \sin \theta = \frac{\vec{k} \cdot \vec{G}}{|\vec{k}| |\vec{G}|} \]  

(2)

In the experiment, if the beam incident angle on the
crystal is not the exact Bragg angle when there is no object,
the reflectivity of the crystal will be changed. So in the
experimental setup, it is essential to have the monochro-
mator and analyzer crystals aligned at their Bragg angle
around the axis (z-axis as shown in Fig. 3) perpendicular to
the plane of diffraction. Also the crystal should be aligned
around a perpendicular axis (x-axis which is along the
beam direction) in the plane of scattering (azimuthal tilt angle). Ideally, there should be no azimuthal tilt angle.
However, it is difficult to achieve and this angle will appear
with time even in an accurate alignment due to thermal or
mechanical drift. Thus the azimuthal tilt angle is referred to

![Synchrotron DEI/MIR experimental setup.](image1)

![Rocking curves.](image2)
as tilt error. Fig. 3 shows the definition of the tilt error $\chi$ in the crystal alignment.

Fig. 4 shows how a fan beam from a point source is reflected by the crystal with a tilt error $\chi$ as would be the case in the DEI experimental setup in a synchrotron facility. A fan beam is used to cover the object in one dimension perpendicular to the median ray; the object is scanned in the other perpendicular direction to form a two dimensional projection image. The crystals are aligned at their Bragg angle $\theta_B$ corresponding to the median ray of the incident beam. This angle must be aligned with sub-microradian accuracy corresponding to the high angular sensitivity of DEI system. The diffraction plane is perpendicular to the crystal lattice plane $XOZ$ and contains the source point, $S$. The presence of azimuthal tilt angle $\chi$ causes intensity variations in the image field, although it is somewhat less sensitive (in 10’s of microradians). The following analysis is for a ray, $SA$, in the fan beam which has an opening angle $\beta$ with the median ray. We will define $\Delta\beta$ as the maximum angular range of the beam, $\Delta\beta = 2\beta_{\text{max}}$, where $\beta_{\text{max}}$ is the maximum opening angle with respect to the median ray.

If there is a tilt $\chi_{m1}$ for the first crystal of the monochromator, the reciprocal lattice vector of this crystal $\vec{G}_{m1}$ represented in the $X$, $Y$, and $Z$ system of Fig. 4 is

$$\vec{G}_{m1} = \frac{1}{d_{hkl}} \begin{bmatrix} 0 \\ \cos \chi_{m1} \\ \sin \chi_{m1} \end{bmatrix}. \quad (3)$$

The wave vector $\vec{k}_{SA}$ of the incident ray $SA$ in the crystal coordinate system also as shown in Fig. 4 is

$$\vec{k}_{SA} = \frac{1}{\lambda_{SA}} \begin{bmatrix} \cos \theta_B \cos \beta \\ -\sin \theta_B \cos \beta \\ \sin \beta \end{bmatrix}. \quad (4)$$

Since the incident ray is polychromatic, the wavelength $\lambda_{SA}$ is selected by the first crystal of the monochromator according to the incident angle on the crystal lattice plane of this ray. This incident angle will be referred to as $\theta_B^\beta$. The wavelength, $\lambda_{SA}$, of this ray can be evaluated if the sine of this angle can be determined. The sine of this incident angle can be represented as

$$\sin \theta_B^\beta = -\frac{\vec{k}_{SA} \cdot \vec{G}_{m1}}{|\vec{k}_{SA}| |\vec{G}_{m1}|} = \sin \theta_B \cos \beta \cos \chi_{m1} - \sin \beta \sin \chi_{m1}. \quad (5)$$

According to the Bragg’s law, the wavelength of this ray is

$$\lambda_{SA} = 2d_{hkl} \sin \theta_B^\beta. \quad (6)$$

The 1st crystal of the monochromator selects the energy for the ray $SA$. The energy selection along $Z'$ axis (from Fig. 4) is shown in Fig. 5 as a function of the opening angle $\beta$ for tilt angles of 0 and $\pm 500$ µr. In the calculation, the crystal is selected as a Si(3,3,3), and is aligned at its Bragg angle for 40 keV. Fig. 6 shows the reflectivity of the 1st
respectively.

This effect is shown in Fig. 7, which narrows down the energy width of the double crystal cause an energy shift of the reflectivity of the 2nd crystal determined by the first crystal. This angular deviation will on the crystal will deviate from the Bragg angle which is in the 2nd crystal of the monochromator, the incident angle in the 2nd crystal of the monochromator as a function of X-ray energy for rays with an opening angle 500 μr.

Fig. 5. Energy selection across the fan beam of the first crystal of the monochromator in the cases of -500, 0, and 500 μr tilt.

crystal of the monochromator as a function of X-ray energy for rays with an opening angle 500 μr at different tilt errors of 0 and ± 500 μr.

The ray is reflected by the 1st crystal of the monochromator in its diffraction plane. Then it is incident on the second crystal of the monochromator and reflected by this crystal in its diffraction plane. When there is a tilt error of the analyzer. Thus, from Eq. (9), we have

\[ \Delta \theta = \theta^B - \theta^A. \]  

(8)

Since the angular shift \( \Delta \theta \), the opening angle of the ray \( \beta \), and all the tilt angles, \( \chi_{m2}, \chi_{m1}, \) and \( \chi_a \), are very small angles, the following approximate relationship is obtained.

\[ \Delta \theta = (2\chi_{m2} - 2\chi_{m1} - \chi_a)\beta / \cos \theta^B. \]  

(9)

This angular change from the Bragg angle will modulate the intensity of the reflected beam in the imaging field according to the rocking curve of the analyzer. The occurrence of the tilt angles will introduce a systematic shift in the rocking curve center and will appear as a linear refraction angle across the field of view (the “β” axis). The tilts from the crystals cannot be separated from each other if only the angular shift of the analyzer rocking curve as a function of \( \beta \) is known. However, by monitoring the rocking curve of the second monochromator crystal one can separate the combined tilt errors of the monochromator crystals from that of the analyzer. It is also seen from Eq. (9) that if the two crystals of the monochromator are tilted in the same way then the effects of the tilts cancel each other, resulting in no net effect as seen by the analyzer. This agrees with intuitive observation that the absolute alignment of the crystals is less important than that of relative alignment between them.

3. Experiments

If there are no tilts between the two crystals of the monochromator, the systematic refraction angle across the fan beam (as a function of \( \beta \)) can be linearly determined by the tilt of the analyzer. Thus, from Eq. (9), we have

\[ \Delta \theta = -\chi_a \beta / \cos \theta^B. \]  

(10)

Since DEI is designed to detect changes in refraction angle, the tilt error of the analyzer can be estimated by the systematic refraction angle derived from the resulting images.
The experiment to verify the relationship between the angular shift of the rocking curve and the tilt error has been done on the X15A beamline at the National Synchrotron Light Source (NSLS) in Upton, New York. In the experiment, the mean beam energy is set at 33.22 keV. The three crystals in the system are Si(3,3,3). The tilt of the analyzer has been deliberately set much larger than what we expect in practice to verify the trigonometric approximations we made in the derivation of Eq. (9). The result is shown in Table 1.

Good agreement was obtained between the induced tilt and the measured values using Eqs. (10) and (11). So the tilt error of the analyzer can be estimated according to the systematic refraction angle found in the images using Eq. (11).

To demonstrate how the above understanding can be applied to practical DEI imaging, images of a set of DEI mammography images taken at different rocking curve points are shown in Fig. 9(a). They were taken at 40 keV on the X15A beamline at the NSLS. The three rocking curves shown in Fig. 9(b) are from three different areas in the bottom of the images where no structured object was present. These three different areas are shown in Fig. 9(a), from left to right marked in squares as A, B, and C. The triangle points on the fitted rocking curves correspond to the analyzer settings (0.5 m from 0 to 3 m).

To be clear, the analyzer positions where the shown images in Fig. 9(a) were taken were marked from 1 to 6 corresponding to image 1 to image 6.

It is obvious that the three fitted rocking curves have different angular shifts. Thus there is a “refraction angle” which is not expected across the image field from left to right. And the effects of this angle can be clearly found in the images. The left region of images taken on the low angle side of the rocking curve is darker than the right region, and vice versa, the right region of images taken on

\[
\chi_a = -\frac{\Delta \theta}{\beta \cos \theta_B}. \tag{11}
\]
the high angle side of the rocking curve is darker than the left region.

The refraction image, $\Delta \theta$, of the top region of the images where no structured object was present was estimated and is shown in Fig. 10(a) as a gray scale image. The averaged profile of the refraction image is shown in Fig. 10(b). The profile can be fitted by a straight line which is also shown in Fig. 10(b). The slope of this line is $-4.26 \text{nrad/mm}$.

At NSLS where the experiments were done, the distance from the source to the detector is 18.65 m. For the analyzer used in the experiment, Si(3,3,3), at 40 keV the Bragg angle is 8.528°. So a tilt error of $\chi = 78.58 \mu\text{rad}$ is found using Eq. (11).

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It is difficult to determine the tilt of the crystals of the monochromator due to the mechanical system which is used to control the tilt angles. However, the compensation of an induced tilt of the 2nd crystal of the monochromator by the tilt of the analyzer can be verified. This compensation is possible as shown in Eq. (9) and occurs when the terms in parentheses sum to zero. This effect has been verified in an experiment also done on X15A imaging beamline at NSLS. In the experiment, the crystals are all Si(3,3,3) and the beam energy was set at 33.22 keV. The images shown in Fig. 11 are rocking curves (vertical direction) across the width of the imaging beam (horizontal direction). These images are derived from several images of the beam as the analyzer is scanned in Bragg angle. The image in Fig. 11(a) is vertically composed of horizontal lines extracted from the vertical center of 101 images taken every 0.2 μrad from $-1$ to 1.5 μrad in analyzer setting around the peak position. The 2nd crystal of the monochromator was misaligned and the tilt of the analyzer was set at $-1.82 \mu\text{rad}$ to achieve compensation. The image shown in Fig. 11(b) is from the same experiment as Fig. 11(a) but tilted in the other direction. The image lines again range from $-10$ to 10 μrad around the peak location in 0.2 μrad.
increments. The tilt of the 2nd crystal of the monochromator was set approximately the same value as in Fig. 11(a) but with opposite sign. A tilt of 1.21 mr of the analyzer is found to compensate the effect of the tilt of the 2nd crystal of the monochromator.

It is also seen from Fig. 11 that even though the angular effect of a monochromator tilt can be compensated perfectly by tilting the analyzer crystal, the intensity variation as a result of a tilted monochromator crystal cannot be compensated. Thus it is still desirable to align the monochromator crystals independently of the analyzer.

4. Corrections of the tilt error in DEI/MIR images

In DEI/MIR image processing, an intrinsic rocking curve of the analyzer is usually estimated from parts of images where no object is present. The parametric images that convey the properties of the object are derived by the comparison between rocking curves from all pixels in the images and this intrinsic rocking curve [1–3]. Obviously, the tilt error complicates the interpretation of the DEI/MIR images by changing the intrinsic rocking curve’s angular location across the image field (“β” axis).
To remove the tilt error, either careful alignment of the crystals is required prior to imaging, or an algorithm will be necessary to remove the effects after imaging. Before imaging, two ion chambers are used to measure the flux emitted from the monochromator and the analyzer, respectively, which are both segmented into two regions about the median ray. The fluxes of these two regions are sampled to make sure that the rocking curve peaks are aligned; if not, the tilt angle is adjusted [9]. However, even if the crystals are exactly aligned at its Bragg angle before imaging, it may drift away during imaging. So it is important to remove the effects of tilt error from the DEI/MIR images by a robust algorithm.

In this paper a method employing multiple reference rocking curves instead of a single intrinsic rocking curve is proposed. The requirement of this method is that there are areas along the beam width where no object is present or reference rocking curves are acquired prior to imaging with the object. These areas can be used to create one reference rocking curve for each column of images by interpolation. In the distillation of parametric images, the current rocking curve is compared to its corresponding column reference rocking curve instead of one single intrinsic rocking curve. The parametric images of the previous DEI mammography images were estimated by the proposed multiple reference rocking curves method. As shown in Fig. 12(b), the tilt error was successfully removed.

Fig. 12. Comparison of the estimated parametric images using different methods. (a) shows images distilled using only one intrinsic rocking curve. (b) shows the parametric images obtained by the proposed multiple reference rocking curves.

Fig. 13. Imaging object and the distilled parametric images with artifacts. (a) is a schematic representation of the object. It is composed of paper sheets, a horizontal lucite rod, and a vertical lucite rod, overlapping from the front to the back. (b)–(d) are the distilled absorption, refraction, and extinction image correspondingly. The parametric images show obvious artifacts, especially on the horizontal lucite rod.
In addition, when there is no tilt, the increment and the range of the analyzer angular settings are determined by the rocking curve, the physical properties of the object, and the sensitivity required in the experiment. When there is a tilt error, the effect of the tilt error has to be considered when the settings in the experiment are determined.

Fig. 13 shows an imaging object and its absorption, refraction, and extinction images distilled from an image set which is acquired when the analyzer had a tilt error 6.06 mr. The angular settings of the analyzer were from $-15$ to $15 \mu r$ about the peak with $3 \mu r$ increments. The artifacts in the parametric images are obvious on the horizontal Lucite rod. This phenomenon is reproduced in the simulation assuming 6 mr analyzer tilt shown in Fig. 14(a) when the object is selected as a vertical rod followed by a horizontal rod. These artifacts are caused by the analyzer steps being significantly larger than half of the Darwin width $\omega_D$ [10]. In this situation there are regions in the image where there is insufficient information to determine the reference rocking curve. The ‘S’ shaped artifacts indicate these regions. When the increment of the analyzer angular settings is decreased to $1 \mu r$, the artifacts are weakened as shown in Fig. 14(b); and when the increment of the analyzer angular settings is further decreased to $0.3 \mu r$, the artifacts can not be detected any more as shown in Fig. 14(c).

The tilted analyzer creates an imaging situation where the reference rocking curve changes in angular location across the image field of view. Thus, if the tilt is large ($\Delta \alpha \geq \omega_D / \Delta \beta \cos \theta_B$) then the DEI analysis method is no longer possible, and the MIR analysis is required to correct the image. The MIR method requires sufficiently dense analyzer settings to be able to determine the object scattering, refraction, and absorption properties. These settings are typically less than $\omega_D/2$ in step size. The case of a tilted analyzer then requires that the scan range be extended so that a sufficient angular range is covered across the field of view. The extension of range should be approximately,

$$\Delta \theta_{\text{ext}} \approx \frac{\Delta \alpha \Delta \beta}{\cos \theta_B}.$$  \hspace{1cm} (12)

5. Conclusions

DEI/MIR requires high precision alignment of crystals in both the Bragg angle and the azimuthal tilt angle. In this paper we present a detailed analysis of the effect of a tilt angle, how it affects the resulting images, and how to determine such a tilt exists. A post processing method employing multiple reference rocking curves instead of one intrinsic rocking curve for distilling the parametric images was implemented and the artifacts caused by the improper angular increment of the analyzer settings is discussed. The result shows that the tilt error can be successfully removed. Estimates have been made of the tilt alignment requirements to achieve the DEI and MIR analysis methods. This information is essential if such systems are to be properly engineered or duplicated. The analysis also applies to multiple crystal systems such as monochromators on

![Fig. 14. Artifacts are weakened with the decrease of the increment of the analyzer angular settings. (a) is the simulation result when the analyzer settings are from $-15$ to $15 \mu r$ with $3 \mu r$ increments with an obvious artifact. (b) is the simulation result when the analyzer settings are from $-15$ to $15 \mu r$ with $1 \mu r$ increments. The artifact is weakened. (c) is the simulation result when the analyzer settings are from $-15$ to $15 \mu r$ with $0.3 \mu r$ increment. The artifact cannot be detected.](image)
synchrotron beamlines, especially for wide horizontal acceptance situations such as bend magnet or wiggler monochromators.

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