Extraction of extinction, refraction and absorption properties in diffraction enhanced imaging

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Received 6 February 2003, in final form 23 May 2003
Published 20 August 2003
Online at stacks.iop.org/JPhysD/36/2152

Abstract
Diffraction enhanced imaging is a radiographic technique that derives contrast from an object's x-ray absorption, refraction gradient and small angle scatter properties (extinction). In prior work, images obtained using two analyser settings were combined to obtain refraction angle and apparent absorption images. A more general method of determining independently the refraction, absorption and extinction of the object is presented. This approach has been used to model the transmission, refraction and scatter distribution of the sample and to visualize these three physical phenomena separately.

1. Introduction

Diffraction enhanced imaging (DEI) is a radiographic technique that derives contrast from an object's x-ray absorption, refraction gradient [1-4] and ultra-small angle scatter properties (extinction) [(5-7), (8)]. Compared with the absorption contrast of conventional radiography, DEI promises to make features in objects more visible by one or some combination of the contrast mechanisms. In DEI, an incident beam is first collimated by a crystal monochromator. This prepared beam is then passed through the object being imaged, and is subsequently diffracted by a crystal that matches the crystals in the monochromator. As DEI was originally applied in [5], the two images obtained using the analyser set to the sides of the rocking curve were observed to contain a mixture of refraction, absorption and extinction information. These two images were arithmetically combined to obtain a refraction angle image with the refraction angle measured in the diffraction plane of the monochromator–analyser system (the vertical direction at the synchrotron). Also an image of the combined absorption–extinction properties was obtained. Due to the limited information contained in two images and the similarity of extinction and absorption, it was not possible to determine these two object properties independently.

The normal procedure for obtaining the refraction angle and apparent absorption image assumes that the peak location of the rocking curve (refraction angle) and amplitude (apparent absorption) can be estimated from the intensity variations on each side of the rocking curve. However, if there is ultra-small angle scattering present, the width of the rocking curve is increased from the intrinsic value and therefore the slope of the rocking curve is decreased. This decreased slope of the local rocking curve where scattering occurs lessens the intensity variations that occur for a given amount of refraction in the object. The lower intensity variations are interpreted by DEI as lowered amounts of refraction. Thus, the presence of extinction affects both the refraction angle and apparent absorption images. In many instances, the enhanced information in these images is sufficient to overcome this mixing of object properties. However, in a more general sense, the independent determination of object properties may play a useful role in identifying structures and features in the object as may be the case in breast cancer [9, 10].
2. Theoretical approach

A possible solution is to make several image measurements of the object at various settings of the analyser crystal in relation to the rocking curve. The intrinsic rocking curve is the reflectivity profile obtained in the absence of the object. From the images of the object obtained at various analyser settings, the centroid of the peak can be estimated that leads to the refraction angle image. This centroid will be un-affected by scattering. The integral of the curve will give an estimate of the absorption losses since the ultra-small angle scattering does not lose x-ray intensity, but only redistributes it into the local (microradian range) region. The parameters that define the amount of scattering and its distribution ($x_s$ and $\omega_S$) can be obtained after the refraction angle and absorption have been corrected for by applying a fit to a simple theory. This analysis is performed on a pixel-by-pixel basis in each of these parameter determinations (refraction angle, absorption, extinction parameters). This method will be referred to as the extinction–refraction–absorption (ERA) analysis.

The scatter mechanism we include in our model has received increasing attention recently. A model-free approach to determining these characteristics, which does not aim specifically to measure $x_{ST}$, was described by us in [11]. The scatter contrast effect was studied empirically in [12]. To apply this model, a method of the object’s absorption, refraction angle and extinction have been developed. To simplify the model, a Gaussian angular distribution and single scattering theory were used. This model simulates the rocking curve observed in a detector pixel through the object with the monochromator–analyser system:

$$R(\theta_A) = e^{-x_{ST}} \int_{-\infty}^{\infty} \left( e^{-x_{ST}} f(\theta) + \frac{1}{\sqrt{2\pi}\omega_S} \left(1 - e^{-x_{ST}} e^{-\theta/2\omega_S}\right) \right. 
\times R_{\text{int}}(\theta - (\theta_A - \theta_1)) d\theta$$

where $R(\theta_A) \equiv I(\theta_A)/I_0$ is the rocking curve (normalized intensity as a function of analyser setting), $\mu_T$ is the linear absorption coefficient, $x_S$ is the extinction coefficient, $t$ is the object thickness and $\theta_1$ is the refraction angle, $\omega_S$ is the Gaussian width of scatter distribution. Note that the intrinsic rocking curve, $R_{\text{int}}(\theta)$ is convolved with the function in brackets to obtain the rocking curve.

This equation contains two parts that embody both a remnant of the direct beam and the developing scattered beam as the thickness of the scatterer increases, as well as an overall attenuation of the transmitted beam due to absorption. The first term in the integral ($e^{-x_{ST}} f(\theta)$) represents the extinction of the direct beam as the thickness increases. As in the case of absorption, this is an exponential decrease in direct beam intensity as the scatterer increases in thickness. The second term now includes the amount of scatter created ($1 - e^{-x_{ST}}$), how this scatter is redistributed in angle ($e^{-\theta/2\omega_S}$), as well as a normalizing factor, $(1/\sqrt{2\pi}\omega_S)$. Since these terms represent the effect on a single ray, the effect in a system with a monochromator and analyser is accomplished by convolving against the intrinsic rocking curve which has included in it the overall refraction of the beam and the specific analyser setting used ($R_{\text{int}}(\theta - (\theta_A - \theta_1))$).

Integrating the rocking curve over all settings of the analyser yields a quantity related only to the total absorption:

$$\Omega = \int R(\theta_A) d\theta_A = \omega_{\text{int}} e^{-\mu_T}$$

where $\omega_{\text{int}} \equiv \int R_{\text{int}}(\theta) d\theta$ (integrated reflectivity of the analyser). This agrees with what we expect from an object that refracts, absorbs and scatters x-rays.

The proposed method is to acquire images at various settings of the analyser in relation to the intrinsic rocking curve and to use the properties of equations (1) and (2) to extract information in the form of refraction angle, absorption, extinction and scattering width.

3. Experimental set-up

The experiments were done at the National Synchrotron Light Source X15A imaging beamline. A schematic of the experimental set-up is shown in figure 1. A monochromatic beam at 18 keV with an energy width of about 2.2 eV was prepared by a two-crystal monochromator using the silicon [3,3] reflection. The analyser used the same reflection in a parallel crystal geometry. These crystals were installed on a one ton granite block to provide stability and minimize mechanical vibrations. The maximum beam size is approximately 5 mm vertical by 125 mm horizontal. We have used a beam size of 1 mm vertical by 60 mm horizontal for these experiments. The sample to be imaged was placed upstream of the analyser crystal. Since the sample is an extended object, it was imaged in a line scan mode to form a two-dimensional image where the motion of the imaging detector and the sample were synchronized. A rotary shutter after the monochromator was used to control the exposure.

A sample (figure 2(a)) was constructed from two crossed Lucite rods (6 mm in diameter) and eight overlapping sheets of paper, in such a way as to produce a variety of combinations of absorption, refraction and extinction effects throughout the image. The Lucite rods produce spatially varying amounts of refraction and absorption, while the arrangement of the paper introduces varying amounts of ultra-small-angle scatter and absorption. The analyser is sensitive only to refraction in the vertical direction; therefore, refraction by the horizontal rod should be visible, whereas refraction by the vertical rod should not.

A total of 24 images of the sample were acquired at 0.8 μrad analyser increments from −9.6 to +8.8 μrad. The measured photon flux was approximately $5.3 \times 10^6$ ph mm$^{-2}$ (1 mGy surface dose in water). A radiograph of the sample

Figure 1. Experimental set-up of a synchrotron based DEI system.
was also taken at a similar exposure after the analyser was removed. The detector was a x-ray photostimulable image plate (Fuji HR-V image plate, Fuji BAS-2500 reader with 50 mm × 50 mm pixel size). Background and scattered radiation on the image plate were reduced by slits in front of the image plate. These slits are set larger than the beam size (approximately 5 mm vertical by 65 mm horizontal) and are used for background reduction during the acquisition time for the 24 exposures on the image plate. In the radiography mode, these background reduction slits were not used since only one image is acquired onto the image plate.

4. Results and discussion

The individual images of the test object were 1256 × 444 pixels (62.8 mm × 22.2 mm) in size. Thus, the image set was composed of 1256 × 444 rocking curves with 24 measured points in each curve. Interactive Data Language (IDL) (Research Systems, Inc.) was used for image processing on a pixel-by-pixel basis to fit the parameters, θ′, μτT, χST and ωS.

The intrinsic rocking curve, Rint(θ), was determined experimentally from the multiple image set and was found to be in agreement with dynamical theory [13]. These data were taken from an unstructured region of the image set away from absorbing, refracting or scattering features.

The refraction angle, θ′, was obtained from the centroid of the sample rocking curve obtained at each point in the image. The absorption, μτT, the extinction, χST and scatter distribution width, ωS, were found by fitting the data on a pixel-by-pixel basis to equation (1) with θ′ fixed according to the previous determination. The iterative fitting routine is based on a gradient-expansion algorithm to compute a non-linear least squares fit to a user-supplied function with an arbitrary number of parameters [14]. The fitting routine required initial estimates of the parameters. These were determined by approximate values. An initial estimate of μτT was based on the use of equation (2),

\[ μτT \approx -\ln \left( \frac{Ω}{ω_{\text{int}}} \right) \]  

where the integrals were replaced by discrete summation of data points.

An initial estimate of χST was obtained by assuming the rocking curve maximum is affected by only absorption and extinction according to,

\[ R(θ_{\text{peak}}) \approx e^{-μτT-χST} \]  

An initial estimate of the scattering width, ωS, was obtained from the full-width half-maximum (FWHM) of the intrinsic rocking curve, ω1 and the measured FWHM at the pixel location, ωR, according to,

\[ ωS \approx \sqrt{ω_1^2 - ω_R^2} \]

Figure 2(b) shows the synchrotron radiograph of the test object that shows very little detail other than the Lucite rods. Two of the images acquired with the analyser at ±1.6 μrad were chosen for DEI analysis [5]. These were chosen at -0.8 and +0.8 μrad. The results are shown in figures 2(c) and (d). Figure 2(c) is the DEI refraction angle image. Figure 2(d) is the DEI apparent absorption image. Figure 3 shows rocking curves along with the fitted curves at various pixel locations within the test object. These locations are indicated in figure 2(a). The A location marks the blank region (no sample) used for obtaining the intrinsic rocking curve. This is shown as the dashed line and has a FWHM of 2.22 μrad. Location B marks a region near the edge of the Lucite rod where the rocking curve is shown as the dash-dot line in figure 3. Note the reduced peak intensity and curve broadening due to the scattering introduced by the 8 layers.

The values of refraction angle, absorption, extinction and scatter width from the multiple image analysis are shown in table 1 for the B and C regions. Figure 4 summarizes the results of the ERA analysis applied to all pixels obtained of the sample. Figures 4(a)–4(d) show the refraction angle image θ′, absorption image μτT, extinction image χST and scatter width image ωS, respectively. The time required to compute this image set was approximately 4 h using a 700 MHz Pentium III personal computer.

The vertical line evident on the left-hand side of figure 4 is due to a monochromator ‘glitch’ which occurs when there

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6 This routine, "CURVFIT", is part of the distribution supplied with IDL (Research Systems, Inc.). This routine is copied from ‘CURVFIT’, least squares fit to a non-linear function.
Here $\Delta$ is the transverse dimension of the object (i.e., the width of the slit in our case), and $\lambda$ is the radiation wavelength. These conditions are satisfied by our parameters, if we avoid the singularity in the first and higher derivatives at the edges of the object. The results of the reconstruction of the maps $\delta(x, z)$ and $\mu(x, z)$, within the framework of the GOA, are presented in figure 3 for an analyser crystal with FWHM of 7°. Figures 3(a) and 3(b) show the initial (reference) maps $\mu^{\text{in}}(x, z)$ and $\delta^{\text{in}}(x, z)$, respectively. These are produced by simulation of attenuation and refraction processes. Figures 3(c) and 3(d) are the corresponding reconstructed maps of $\mu^{\text{rec}}(x, z)$ and $\delta^{\text{rec}}(x, z)$, respectively. The quality of the reconstructed images can be quantified by using the following root mean square parameters:

$$
\Phi^{\mu} = \left[ \frac{1}{N} \sum_{i=1}^{N} (\mu_i^{\text{in}} - \mu_i^{\text{rec}})^2 \right]^{1/2},
$$

$$
\Phi^{\delta} = \left[ \frac{1}{N} \sum_{i=1}^{N} (\delta_i^{\text{in}} - \delta_i^{\text{rec}})^2 \right]^{1/2}.
$$

The values of the parameters $\Phi^{\mu, \delta}$ are presented in table 1. Errors in the reconstructed images occur along the boundary of the cylinder (see figure 4). There are two sources of these errors. The first is due to the rapid phase change near the boundaries, while the second error results from the averaging over the slit width. The regularization procedure takes into account the second derivative and can partly correct for the first kind of error. Decreasing the second kind of error can be achieved by reducing the slit width and the sampling step; however, this increases the measurement time and has restrictions (see equation (11)). However, in principle the restrictions imposed by the GOA can be relaxed, allowing a reduction in both kinds of error. This is the subject of on-going work.

Table 1. Summary of the root mean square parameters for the maps $\delta(x, z)$ and $\mu(x, z)$.  

<table>
<thead>
<tr>
<th>Method</th>
<th>$\Phi^{\mu}$</th>
<th>$\Phi^{\delta}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GOA (FWHM of 5°)</td>
<td>$2.77 \times 10^{-7}$</td>
<td>32.5</td>
</tr>
<tr>
<td>GOA (for FWHM of 7°)</td>
<td>$2.44 \times 10^{-7}$</td>
<td>20.9</td>
</tr>
<tr>
<td>After regularization</td>
<td>$2.29 \times 10^{-7}$</td>
<td>19.4</td>
</tr>
</tbody>
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Figure 3. Reconstruction of the maps $\mu(x, z)$ (in m$^{-1}$) and $\delta(x, z)$ within the framework of the GOA: (a) and (b) are the initial maps $\mu^{\text{in}}(x, z)$ (in m$^{-1}$) and $\delta^{\text{in}}(x, z)$, respectively, used for the simulation of attenuation and refraction processes; (c) and (d) are the reconstructed maps $\mu^{\text{rec}}(x, z)$ (in m$^{-1}$) and $\delta^{\text{rec}}(x, z)$, respectively.
improving visualization of a class of materials invisible to radiography.

In this study, we have used a data set comprising 24 images at various analyser settings. We are presently assessing how many images, their location in analyser angle and the dose or flux required for each to determine the refraction, absorption and extinction parameter with some degree of statistical accuracy. These studies will ultimately determine how this method may apply to various types of imaging problems especially with regard to possible medical applications. At present, since most of our studies focus on inert objects (test objects as in this study, human and animal tissues and materials imaging) the dose and time required for these analyses is not an issue.

Acknowledgments

The authors would like to acknowledge the support of NIH/NIAMS grant R01 AR48292 (MW, DC), NIH/NIGMS grant R21 GM59395-01 (MH, OO, DC), and the US Army MRMC grant DAMD17-99-9217 (DC). The National Synchrotron Light Source, Brookhaven National Laboratory, is supported by the US Department of Energy, Division of Materials Sciences and Division of Chemical Sciences, under Contract No DE-AC02-98CH10886. In addition, we acknowledge the support of the State of Illinois Higher Education Cooperative Agreement.

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