BNL-224001-2023-JAAM

Optical Design of DEI/ABI System at the HEX Beamline at the NSLS-II

Z. Zhong

To be published in "Synchrotron Radiation News"

November 2021

Photon Sciences

Brookhaven National Laboratory

U.S. Department of Energy

USDOE Office of Science (SC), Basic Energy Sciences (BES) (SC-22)

DISCLAIMER

Optical Design of DEI/ABI System at the HEX Beamline at the NSLS-II

Z. Zhong[1], A. Broadbent[1], M. Drakopoulos[1], J. Dvorak[1], M. Hasnah[2], D. Holmes[3], M. Lucas[1], S. O'Hara[1], E. Softye[1], A. Wang[4*]

1. National Synchrotron Light Source II, Brookhaven National Lab, Upton, NY 11973, USA
2. Department of Mathematics, Statistics and Physics, Qatar University, Al Jamiaa St, Doha, Qatar
3. FMB-Oxford, Unit One Ferry Mills, Osney Mead, Oxford OX2 0ES, UK
4. Half Hollow Hills High School East. 50 Vanderbilt Pkwy, Dix Hills NY 11746, USA

* High school students volunteering at the HEX beamline of NSLS-II

Abstract

Diffraction Enhanced Imaging (DEI) or Analyzer Based Imaging (ABI) uses a perfect crystal monochromator and matching analyzer to achieve sensitivity to x-ray refraction and ultra small-angle scattering on the order of 0.01 micro-radians. As such, a thermal bump caused by heat-load in the order of 1 W is detrimental. The heat load at the HEX (High Energy Engineering X-ray) super-conducting wiggler (SCW) beamline, under construction at the NSLS-II, is on the order of 1 kW. How to reconcile the three orders of magnitude difference between the HEX source power and the DEI/ABI requirements?

The solution involves using a double-crystal bent-Laue monochromator as pre-monochromator to prepare a beam with a large divergence and bandwidth that is matched to a flat crystal [333] post-monochromator.

We show through phase-space (x-ray energy vs. angle as viewed by a flat crystal) analysis and Dumond diagrams that there is indeed a unique bending radius that matches the double-crystal bent-Laue monochromator in phase space to the flat Bragg crystal. The matched system has a desirable feature that the phase space of the bent crystal's output beam is much larger than that of the flat crystal, making the combined system stable. Based on these considerations, we present our optical design for performing DEI/ABI at the HEX beamline.

DEI/ABI

DEI/ABI introduces fine selectivity for the angular deviation of X-rays traversing the subject. Since its inception at the National Synchrotron Light Source (NSLS) in the mid 1990s, DEI beamlines have been implemented at a half dozen synchrotron facilities around the world. In 2008, we reported in Synchrotron Radiation News the status of DEI at the NSLS, advancement in DEI instrumentation using an x-ray tube as the source of x-rays and its potential for Alzheimer's disease research [1]. Since then, DEI was shown to be advantageous in areas of radiology of clinical relevance, including breast, lung, cartilage and brain imaging [2-8].

In DEI, a collimated monochromatic x-ray beam is passed through the subject. A silicon crystal (analyzer) is placed between the subject and the detector. The analyzer, with its narrow angular reflection width of a few microradians, provides the ideal tool to analyze, on the micro-radian scale, the angular distribution of x-rays traversing the subject (Figure 1a).

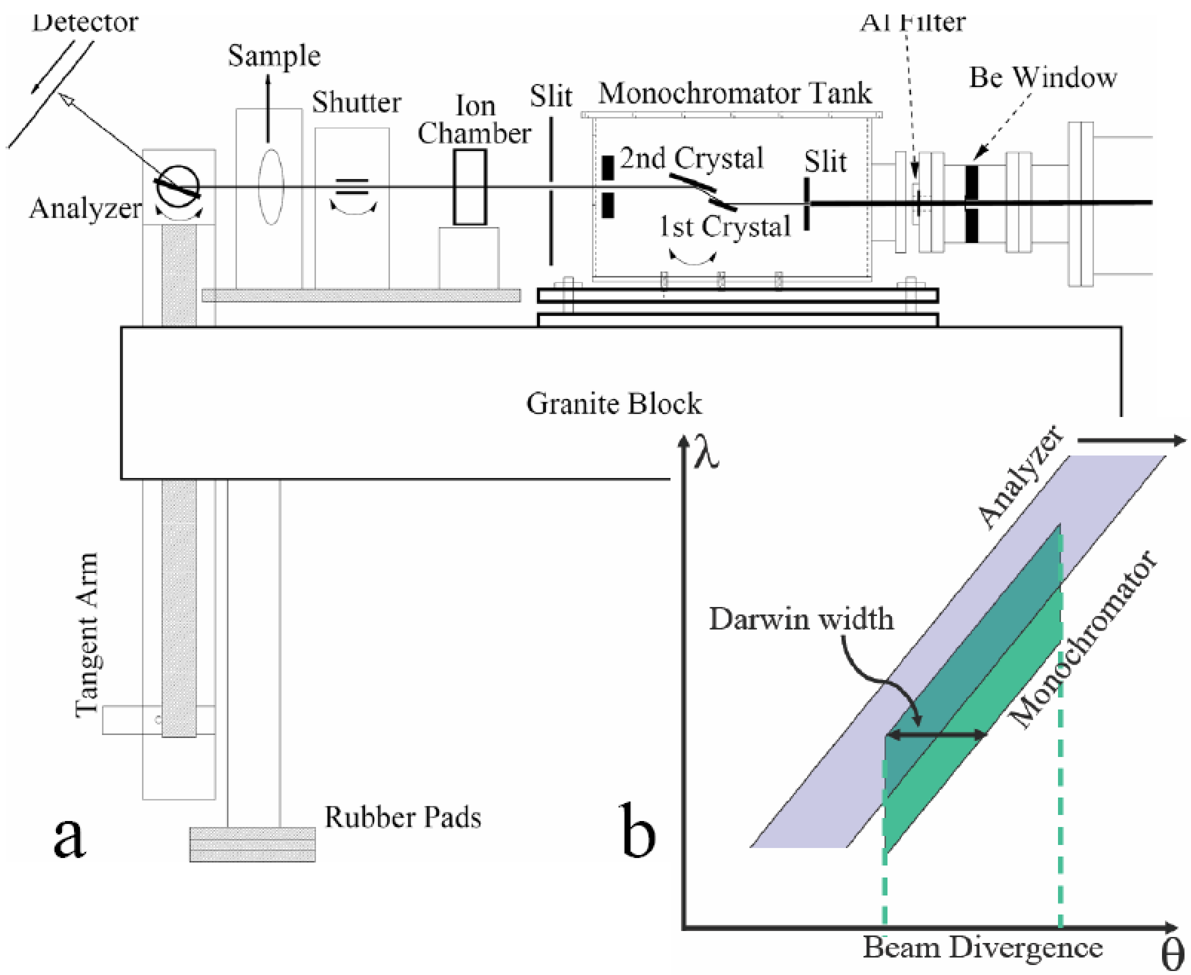

Figure 1. a) DEI setup at the X15A beamline. b) Dumond diagram showing that the perfect crystal [333] monochromator creates a beam of a few micro-radians in divergence in the phase space, regardless of the incident beam divergence, which is analyzed by a non-dispersive perfect crystal [333] analyzer.

Ultra-small angle scattering arises from x-ray diffraction from structures. This scattering intensity is rejected by the analyzer crystal, creating a detectable intensity change (extinction contrast). Also, density variations in the subject refract the x-rays by sub-microradians. The analyzer converts these subtle angle variations into intensity changes (refraction contrast) [2]. Thus, DEI introduces two new sources of image contrast: refraction and extinction (Figure 1b). Both enhance soft-tissue imaging, which lacks contrast in traditional x-rays and CT. the DEI contrast mechanism has been shown to be applicable in both planar [2] and CT modes [3].

As was mentioned in our previous SRN article [1], water-cooling was added to the second crystal of the X15A monochromator to ensure temperature matching between the two crystals. This was done as a necessity after we discovered that the previous system drifts by about a tenth of a microradian over the course of a few hours. This highlights the fact that DEI/ABI, being sensitive to sub-microradians refraction, can tolerate very little heat load.

At the NSLS X15A bending magnet beamline, we had to filter the white-beam with 2 to 5 mm of aluminum, reducing the power on the first crystal to about 1 Watt, to make the head-load manageable. In fact, while performing DEI CT experiments at the NSLS-II in the early 2000s, we found that the heat emitted by the stepper motor of the sample stage, about 1 m away from the analyzer, impacts the performance of the analyzer enough that we went through the trouble of water-cooling the stepper motor (Fig.2).

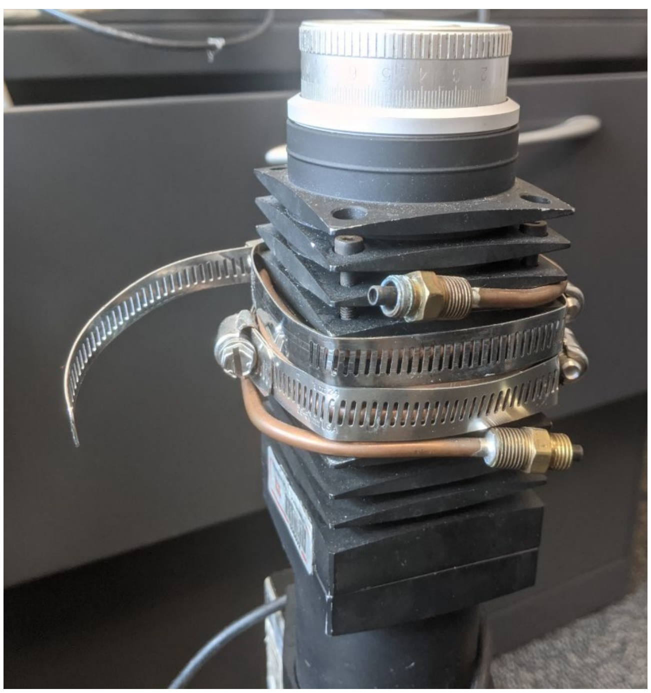

Figure 2. Water-cooling of the sample translation motor to stabilize the analyzer crystal at X15A.

NSLS was shut down in 2014 to be replaced by the NSLS-II. We are currently designing and constructing the HEX beamline at the NSLS-II. The source of HEX is a superconducting wiggler which provides a beam that is 20 mm high and 100 mm wide at the experimental hutch F at 100 m from the source. This is perfect for biomedical and industrial imaging with DEI/ABI in many aspects: large beam size, high energy enabling low dose imaging to take full advantage of the phase contrast, and high flux allowing for fast imaging.

There is one problem to the obvious solution of simply taking the DEI system from NSLS X15A and putting it in the HEX white beam: the heat load. The thermal bump of the first crystal must be kept below a fraction of the monochromator and analyzer's Darwin width, which is 0.8 micro-radians at 60 keV for Si [333]. The power load on the first Bragg crystal of the monochromator is 1.2 kW assuming 6 mm of diamond and 4 mm of SiC filtering. The thermal bump makes a Bragg perfect crystal in the HEX white beam, as shown in Fig.1a, difficult if not impossible. A new solution is needed.

Bent Laue Monochromator

HEX is designed with a high-energy non-focusing x-ray monochromator for full-field imaging. High-energy x-rays are especially suitable for imaging batteries, engineering materials, earth science samples as well as biomedical subjects. Simulations show that bent-Laue crystal monochromator can be used at HEX to provide high-energy x-rays at a flux on the order of 10^{11} ph/s/mm^2. The monochromatic beam size can be reduced by the use of slits to allow for Angle Dispersive X-ray Diffraction (ADXD).

The HEX Laue monochromator consists of two nearly identical bent crystals with the first crystal being cryogenically cooled. Both crystals have pitch angular adjustment and the second crystal can be translated along the white-beam direction to allow for energy change while maintaining a fixed exit beam height. Fig. 3 shows schematically the design of the imaging monochromator.

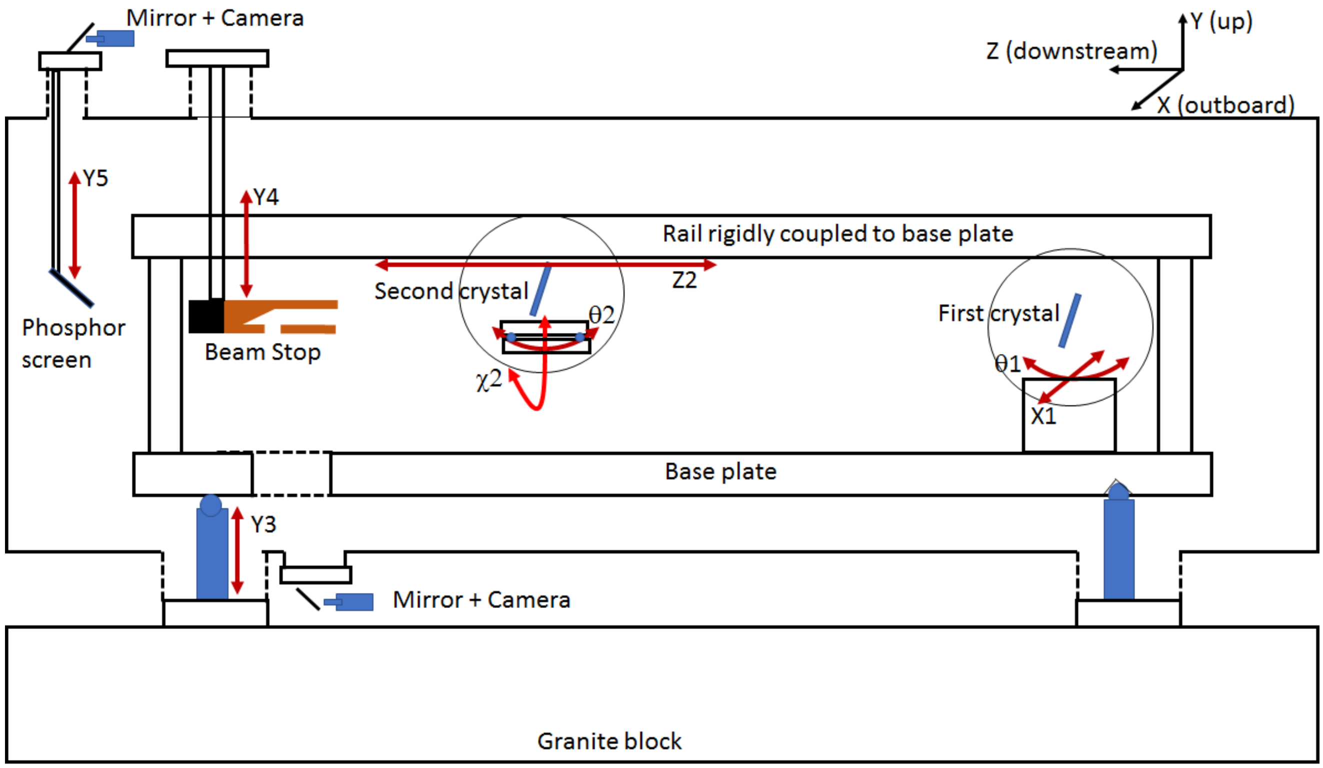

Figure 3. Key design elements and motions of the HEX monochromator

The following design ideas apply to the imaging monochromator:
1.The HEX center branch, which the monochromator serves, is white-beam compatible. Thus, a small offset of 25 mm is chosen to minimize the distance between the two crystals and between the monochromatic and white beam heights. This affords a compact design and higher stability.
2. The first crystal is cryogenically cooled by liquid nitrogen to enhance thermal stability.
3.The first crystal and beam stop are removable from the white beam to allow white-beam operation.

The monochromator is located in the First Optical Enclosure with the following parameters: Source to monochromator distance is 31 m; monochromator to sample distance is 73 m. It provides a large (100 mm x 20 mm) field of view at the F-station in the satellite building outside of the storage ring building. The x-ray energy provided by the monochromator is variable between 30 and 150 keV.

The monochromator crystal design choice involves a large parameter space that includes the reflection chosen, asymmetry angle, crystal thickness, and bending radius. The above factors also depend on the desired operating x-ray energy. Generally, a larger asymmetry angle results in higher bandwidth and higher flux. However, if the asymmetry angle is too large, the beam footprint on the crystal increases. A thicker crystal results in larger bandwidth and higher flux at high x-ray energy. However, thicker crystals affect performance at low x-ray energy due to the crystal's self-absorption.

To explore the parameter space to guide an intelligent choice of crystal parameters that suit the unique requirement for imaging at the HEX beamline, an IDL program was written, using the lamella model for bent-crystals, to explore the parameter space.

Fig. 4 shows the result of the optimization at 50 keV for various imaging monochromator parameters: asymmetry angle, thickness, and bending radius. The reflection used is silicon [111]. The figure of merit (FOM), represented by grayscale in this figure (lighter color means higher FOM), is the reflectivity multiplied by the integrated reflectivity in milli-radians. This FOM is proportional to the output flux of the two-crystal monochromator system.

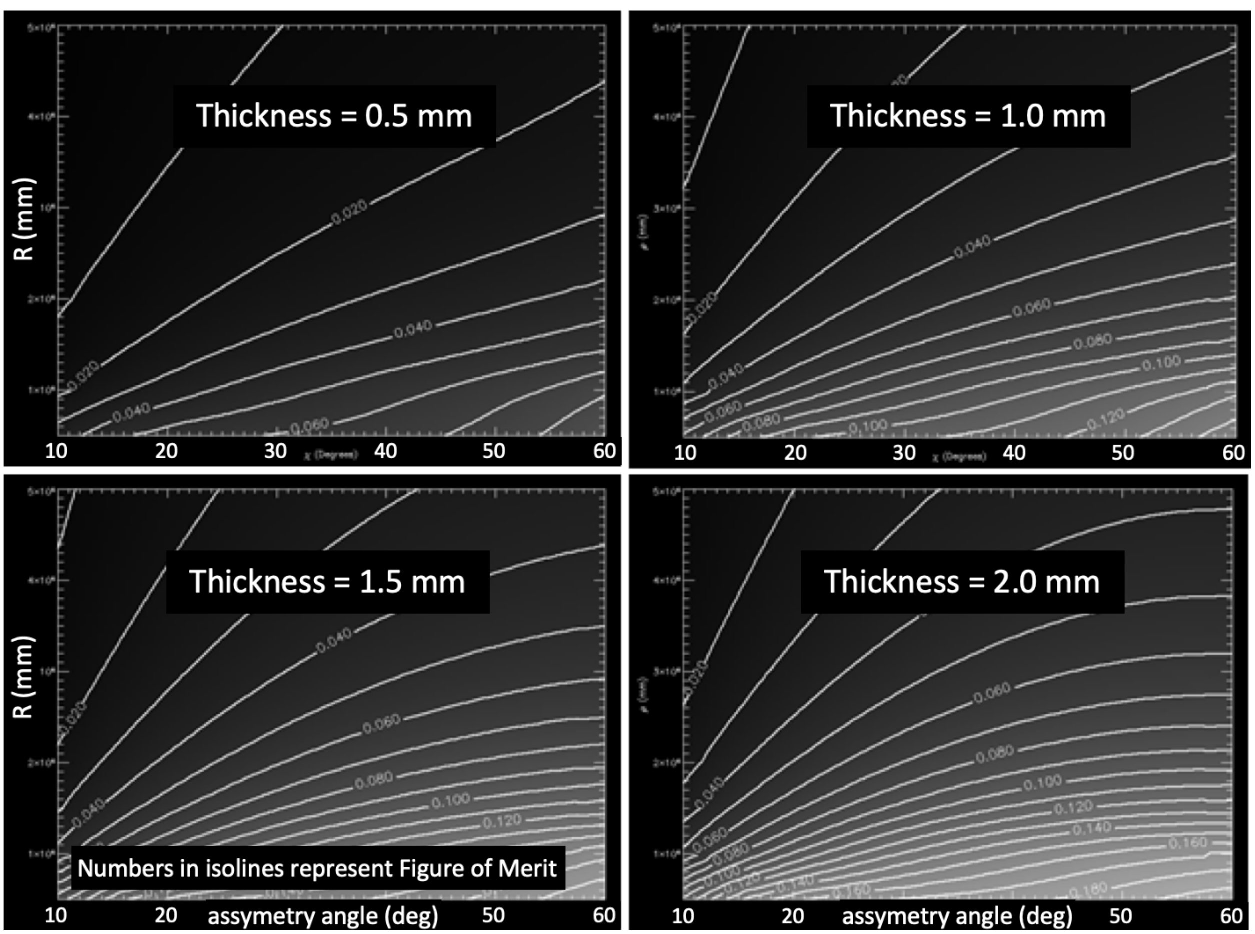

Figure 4. Result of the optimization at 50 keV for various imaging monochromator parameters: asymmetry angle, thickness, and bending radius. The grayscale and isolines represent a figure of merit proportional to the output flux of the monochromator.

Similar simulations were performed at 30 and 150 keV to assess the effects of the parameters on the performance across the desired energy range.

Analysis of optimization results shows that the benefit of larger asymmetry angle levels off after about 40 degrees. Therefore, the symmetrical crystal cut at a 35.3 degrees asymmetry angle for the [111] reflection, with crystal surface being <100>, shown in Fig.5, is an appropriate choice.

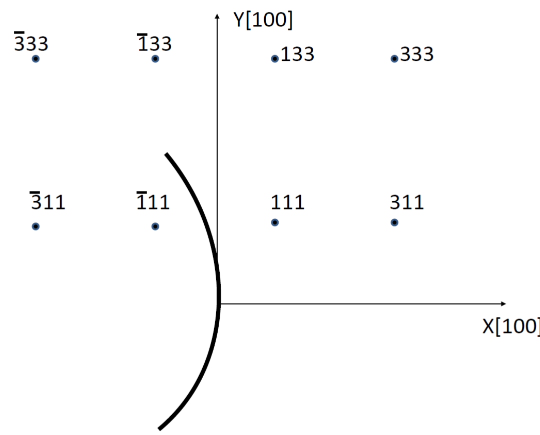

Figure 5. Reciprocal space configurations of a Laue crystal with the surface normal being 100, and the 111 reflection at 35.3 degrees asymmetry angle

The advantages of a 100 crystal are:

1. Simple symmetrical crystal design minimizes confusion. For example, accidental or deliberate flipping of the crystal would have no negative consequences.
2. The [111] reflection provides high flux for imaging and no second harmonics.
3. On the same crystal, it is shown in Fig. 5 that the [022] is a symmetrical reflection with 0 asymmetry angle. At 0-degree asymmetry angle, bending the crystal generally does not broaden the rocking-curve width. This reflection is a thus good choice for a very high resolution, and consequently lower flux, beam.
4. The [311] reflection on the same crystal has high resolution and moderate flux, with no second harmonics. This reflection is a good candidate for diffraction studies that require high resolution.

We note that the [022] and [311] reflections, both about 30 degrees from nominal [111] position, require a goniometer with a large angular range of about 70 degrees to be accessible.

As for the choice of crystal thickness, the optimization studies show that 1.5- 2 mm allows reasonable 30 keV performance, while thicker crystals benefit higher energies. We choose 2 mm nominal thickness for the first and second crystal in our baseline design due to the desire to image at 30 keV. According to the lamellar model, as a result of the systematic change of the angle of the lattice plane from the front to the back of the crystal along the beam path, the bent-Laue crystal's reflectivity profile is typically rectangular in shape. The rocking curve between two identical crystals is the convolution of two rectangles, resulting in a triangular rocking curve. Operating the monochromator with a triangular rocking curve results in intensity fluctuations as the relative angle between the crystals changes. Since the rocking curve width is proportional to the crystal thickness, if the second crystal is slightly thicker than the first crystal, then the rocking curve would be a trapezoid, resulting in better intensity stability of the monochromatic beam. Thus, the second crystal has a slightly larger thickness (2.2 mm, 10% above nominal) than the first crystal (1.8 mm, 10% below nominal) to achieve a flat-top in the rocking curve. This concept was successfully implemented by the MECT monochromator at X17B beamline of the NSLS.

As expected, a smaller bending radius results in higher flux at the cost of a larger energy difference between the top- and bottom- parts of the beam. The flux benefit levels off at radii smaller than 10 m.

The monochromator was constructed and assembled recently. Fig. 6 shows a photo of the first crystal, the bender consisting of two leaf-springs, and the cooling arrangement. The thin region in the middle is used for diffraction. The crystal is cooled by clamping the cooling block on the thick part of the crystal, minimizing the propagation of stress to the active region.

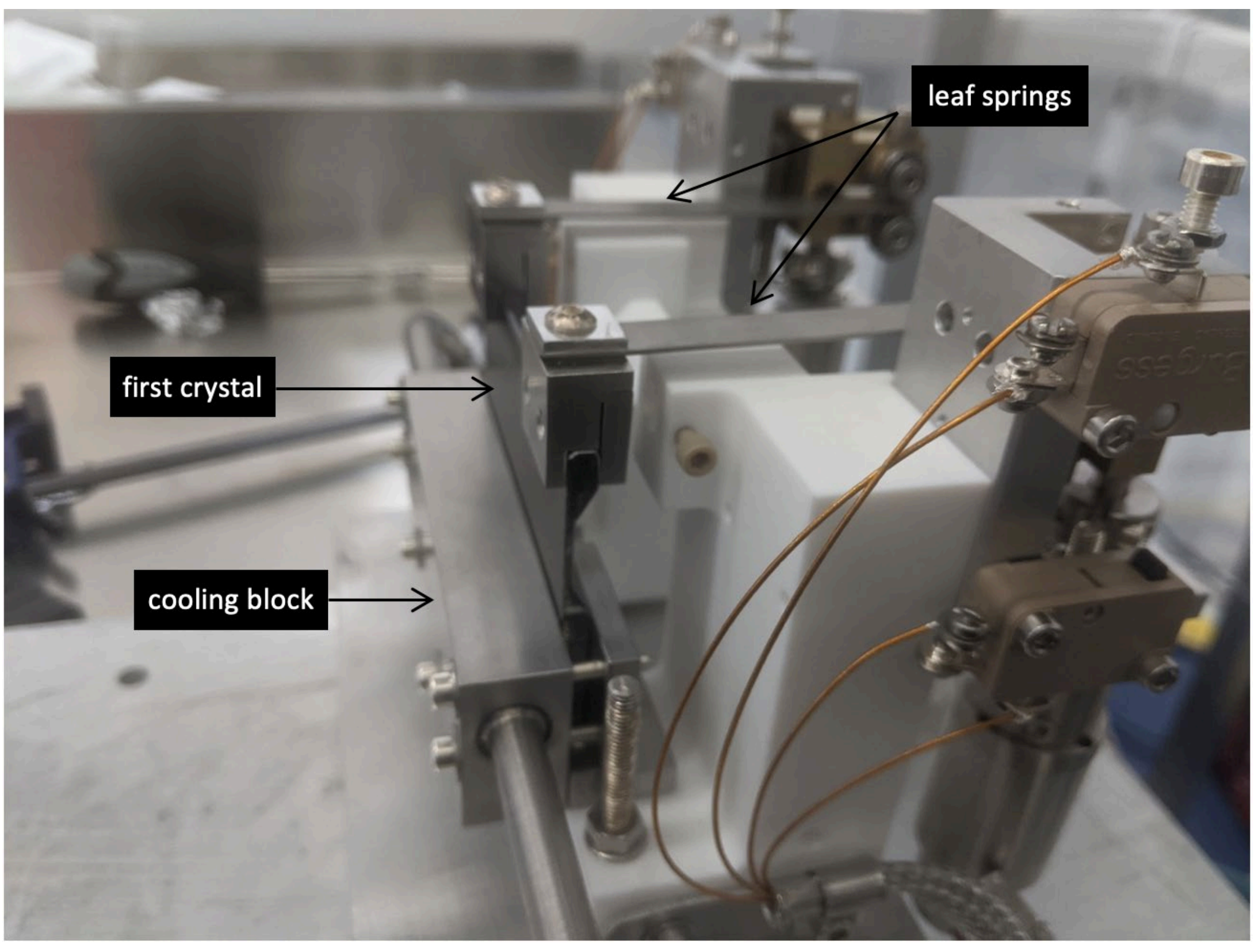

Figure 6. Photograph of the first crystal and its bender.

Phase Space Matching Between Flat [111] and [333] crystals

The phase-space of a perfect flat crystal is well understood and is best depicted with the Dumond diagram. Figure 1 shows the Dumond diagram of the 111 reflection, typically used by monochromators for diffraction and spectroscopy, and of the 333 reflection, typically used for DEI due to its much narrower rocking-curve width. Using analytical formulas based on dynamical theory of x-ray diffraction, a software code was written using IDL programming language to simulate and display the Dumond diagram (Fig. 7). The HEX vertical angular divergence of 200 micro-radians was assumed for the simulation. An X-ray energy of 30 keV is assumed.

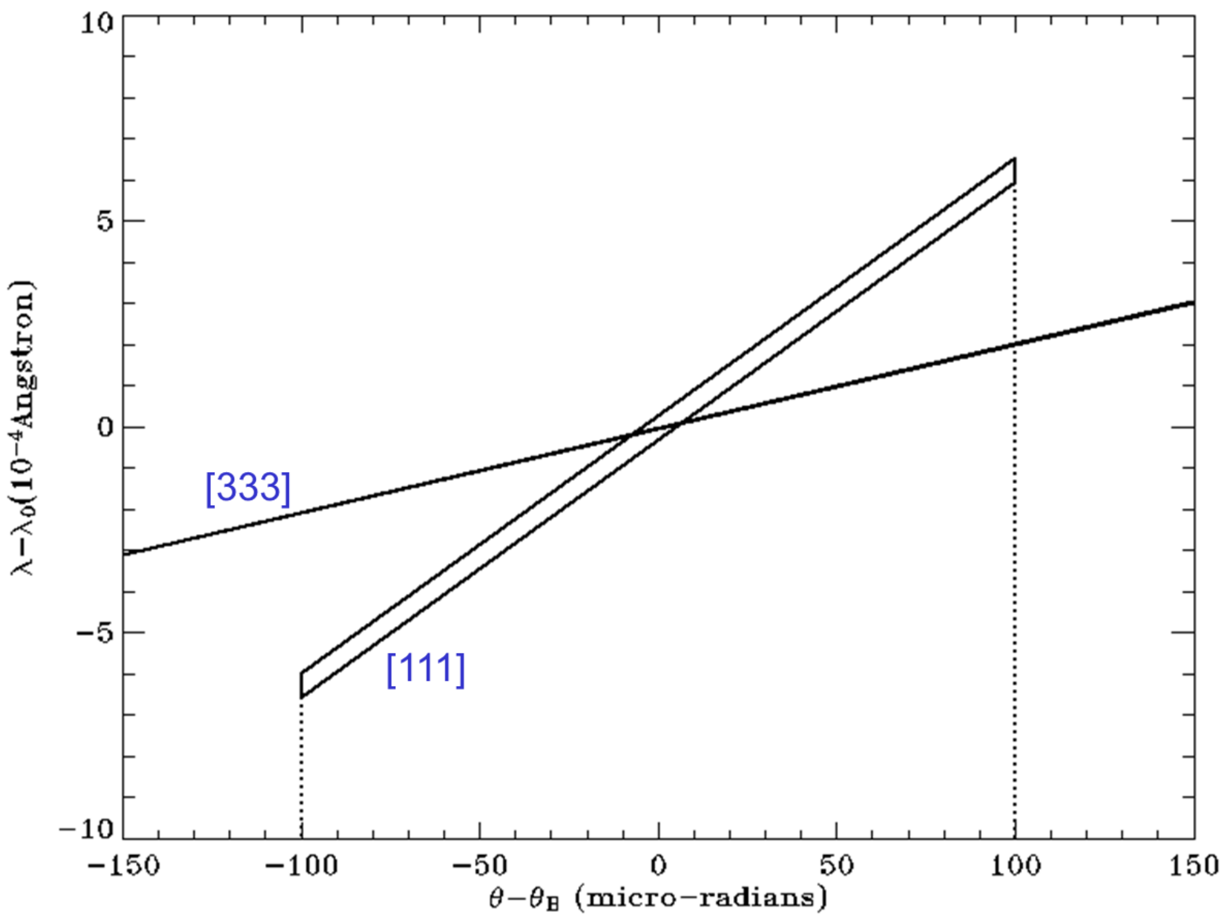

Figure 7. Dumond diagram of a two-crystal system consisting of a perfect crystal with 111 reflection and a perfect crystal with 333 reflection.

It is seen that the vertical divergence of the beam dominates the bandwidth of the output beam. The intrinsic Darwin width is smaller in comparison, especially for the 333 reflection. For each phase space, the horizontal width is the Darwin width. The slope is $2d\cos(\theta)$, where d is the d-spacing of the reflection. We note that there is little overlap, about 15 micro-radians, between the 111 and 333 reflections. This means that if we attempt to perform ABI or DEI with a Bragg [333] reflection by simply unbending the Laue crystals using [111] reflection , the beam for phase-contrast imaging will only be 15 micro-radians in divergence compared to the 200 micro-radians divergence of the incident beam, thus more than 90% of the beam will be lost. This highlights the importance of matching crystals in phase space, and also suggests that simply making both crystals in the monochromator flat will not provide an optimum beam for DEI implementation. A better solution is needed.

Phase Space Matching Between [111] Bent-Laue and [333] Perfect Bragg Post-monochromator

For performing the DEI experiment, we plan to deliver the double bent-Laue beam into the experimental hutch F, and then use a [333] perfect Bragg crystal as a post-monochromator as shown in Fig.8. Both Laue crystals are typically bent towards the source to minimize the energy difference between the top- and bottom- parts of the beam. The change in divergence after the first crystal is compensated for by the second crystal so that the virtual source size remains (almost) unchanged after the second crystal. The post-monochromator, having near-zero heat load, will then be ideally matched to a perfect Bragg [333] analyzer. [333] is necessary for DEI to achieve high sensitivity to phase contrast.

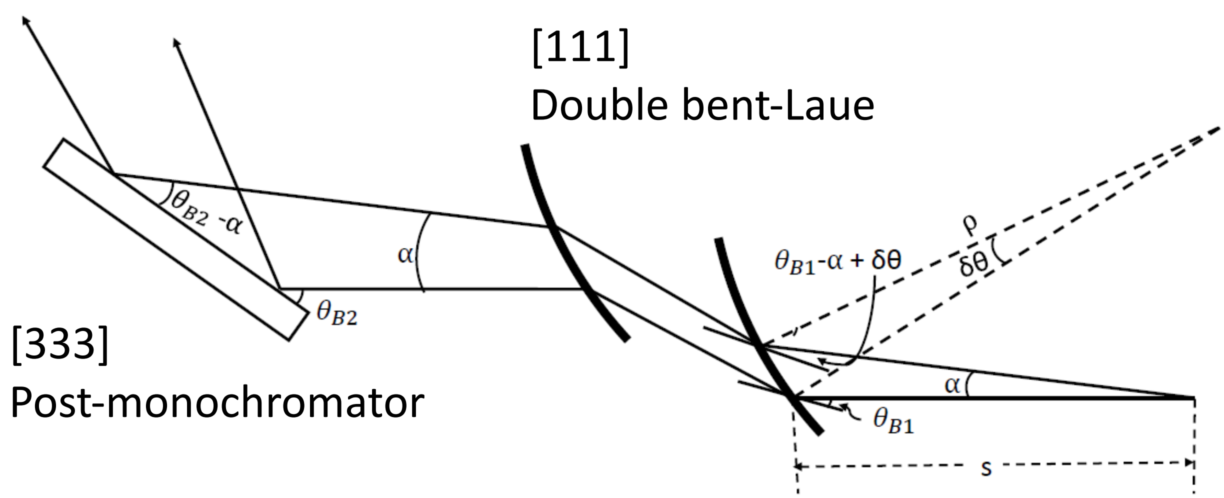

Fig.8 Schematic representation of a system consisting of a double bent-Laue monochromator and a flat Bragg post-monochromator

The condition for phase-space matching a double-crystal Laue monochromator with a perfect Bragg flat crystal is described in [9]. A summary of the conclusion is presented here.

From Fig. 8 it can be derived that the wavelength of the beam at an angle α relative to the central ray is

$\Delta\lambda_1 = 2\Delta\theta_{B2}\, d_1\cos\theta_{B1}$

Where d_1 and θ_{B1} are the lattice spacing and Bragg angle, respectively, of the [111] reflection. The output beam maintains the same divergence as the incident beam for the double-crystal monochromator. The subsequent flat Bragg crystal is oriented to the same Bragg-angle as for the center rays of the two Laue crystals (Figure 5). Thus, the deviation of the extremal ray from the Bragg angle is

$\theta_{B2} = -\alpha$

Assuming that the Bragg crystal diffracts the beam, the deviation of the wavelength from the center ray wavelength $\Delta\lambda_2$ is
$\Delta\lambda_2 = -2\alpha\, d_2\cos\theta_{B2}$

Requiring $\Delta\lambda_1$ to be the same as $\Delta\lambda_2$ results in the bending radius that allows the phase space of the Bragg pre-monochromator to match that of the double-Laue monochromator

$$\rho = s\frac{d_1\cos\theta_{B1}}{cos(\chi - \theta_{B1})(d_1 cos\theta_{B1} - d_2 cos\theta_{B2})}$$

For the special case where both crystals use the same reflection, the solution is that ρ is infinity, meaning that the Laue crystals are un-bent. This is the +-+ (non-dispersive) condition [10,11] for flat crystals.

Consider the HEX case where the first two bent-Laue crystals use the [111] reflection and the post-monochromator uses the [333] reflection. In this case $d_1 = 3d_2$. Applying the approximation that $\cos\theta_{B1,2}\approx 1$, the bending radius for phase-space matching is then

$$\rho = \frac{3s}{2cos(\chi - \theta_{B1})}$$

To gain intuition into the above analysis, Dumond diagrams were used to illustrate matching. Figure 9 shows the Dumond diagrams of the phase space (from the point of view of the flat [333]crystal) of the output beam from a double-crystal bent Laue monochromator at 30 keV. We define $\rho_c = s/\cos(\chi - \theta_{B1})$, the bending radius of the inverse Cauchois geometry. Both Laue crystals are assumed to be using 111 reflection bent to $\rho_c/2$, ρ_c, $3\rho_c/2$, and infinity (flat [111]). The [333] flat crystal's phase space is also shown. The HEX monochromator parameters (thickness = 1.8 mm, asymmetry angle is 35.3 degrees, source-to-monochromator distance s =32 m) is used for generating the diagram.

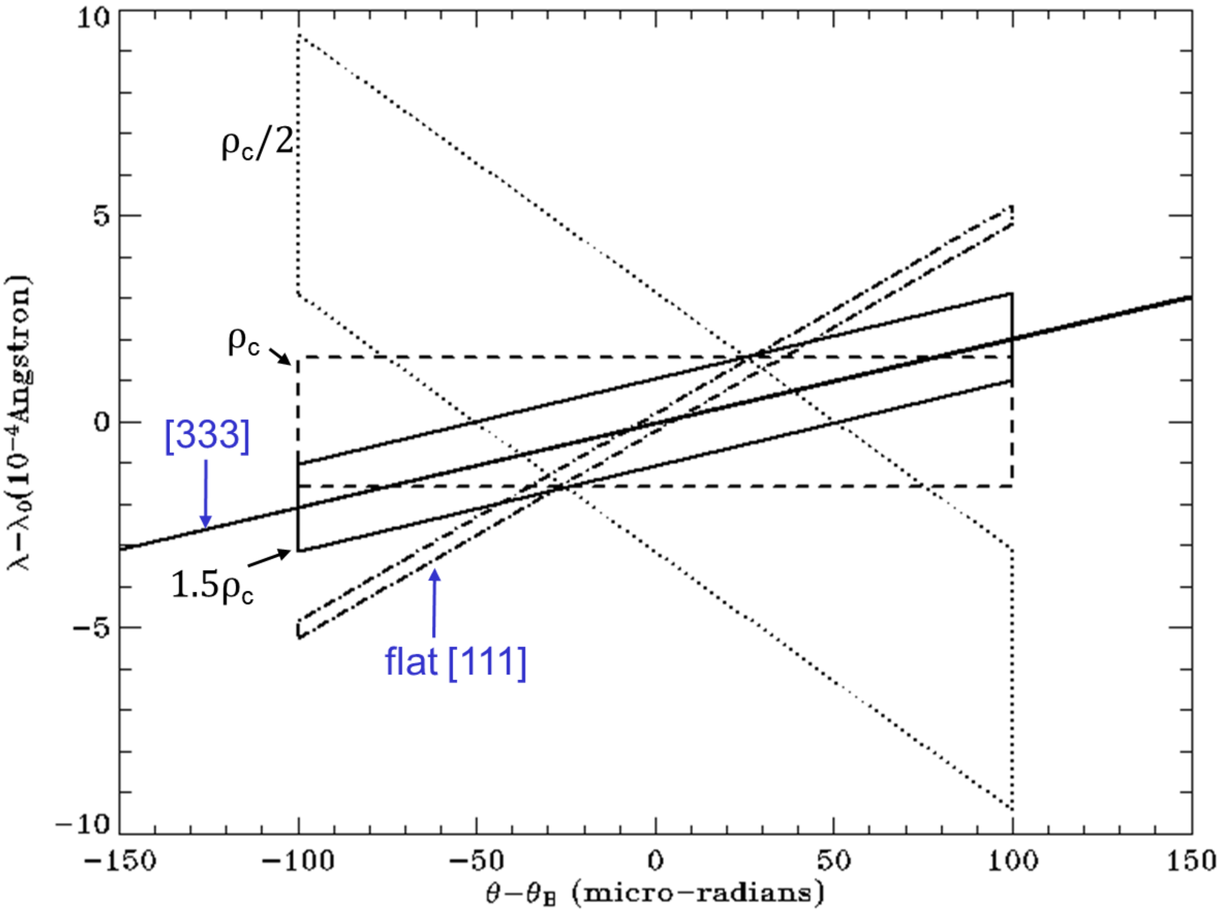

Figure 9. Dumond diagram for the bent-Laue monochromator and post-monochromator system shown in figure 8, with the monochromator crystals being flat and bent to representative radii of 0.5ρ_c, ρ_c, 1.5ρ_c.

Figure 9 shows that at 56.3 m (1.5ρ_c) bending radius there is perfect matching between the phase space of [333] perfect crystal and the double-crystal bent Laue-Laue monochromator. As expected, the output beam of the [333] Bragg crystal has a divergence of 200 micro-radians, same as that of the beam produced by the double-Laue monochromator.

As shown in Fig.9, unless the crystals are bent to a radius of 1.5ρ_c there is a phase space mis-match resulting in loss of beam size and intensity. This confirms the conventional wisdom that if one puts a perfect crystal in a beam produced by a bent-Laue crystal, one usually gets a small beam due to phase-space mismatch between the two classes of optics.

Using the lamellar model, the FWHM for the bent Laue crystal reflection is 42 micro-radians. This suggests that DEI can be implemented at HEX using double bent-Laue monochromators with excellent intensity stability.

Summary

Diffraction Enhanced Imaging (DEI) or Analyzer Based Imaging (ABI) is a powerful X-ray imaging technique that provides significantly higher contrast than conventional absorption contrast in soft tissue, and therefore has important applications in medical imaging. However, it relies on microradian sensitivity to beam divergence, and therefore is difficult to implement without significant loss of throughput on high heat load beamlines due to thermal distortions on the monochromator. The HEX (High Energy Engineering X-ray) beamline has a superconducting wiggler source, which supplies an incident power ~1.3 kW to the monochromator. This presents a significant challenge. The challenge is met by phase-space analysis of the bent-Laue monochromator at HEX resulting in a unique bending radius. When bent to the correct radius, the Laue monochromator produces a beam that covers the phase-space of the [333] Bragg post-monochromator.

To perform DEI at HEX, we plan to place a [333] double Bragg crystal post-monochromator in the F station and place the analyzer behind the post-monochromator +-+ arrangement and position the sample between the two Bragg crystals. The experimental configuration is shown schematically in Fig.10.

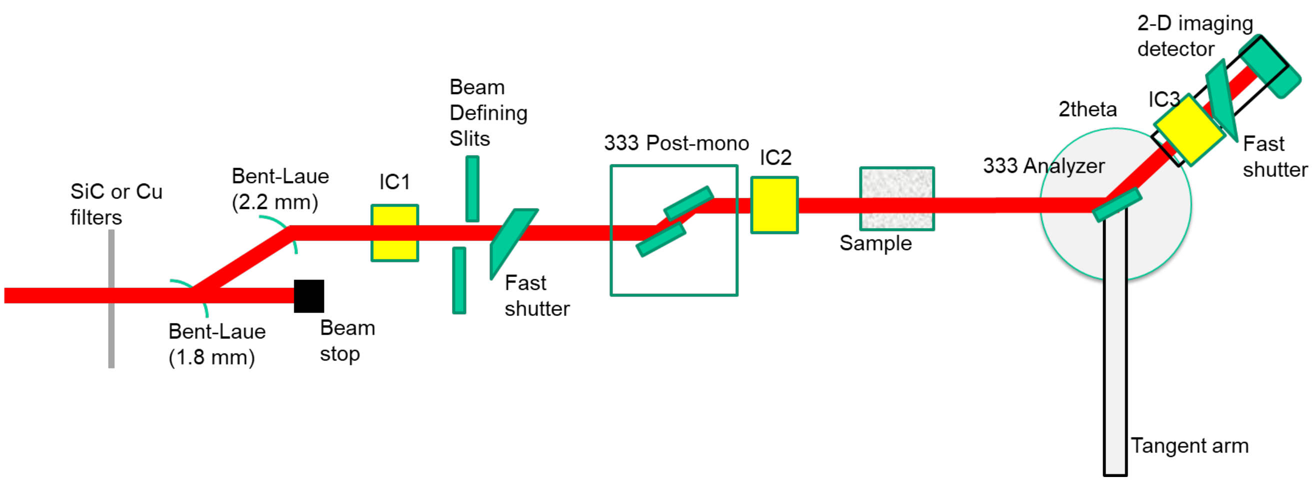

Figure 10. Optical design for DEI/ABI imaging. A [333] double Bragg post-monochromator and a [333] Bragg analyzer are placed in the F experimental station.

Despite the large divergence of the incident beam, the rocking curve of the analyzer crystal will be triangular with a narrow FWHM (Full Width at Half Maximum) of approximately 1.9 micro-radians at 30 keV. The idea of realizing a narrow rocking curve, which enables DEI, with a pair of 333 crystals in a beam with much larger divergence is illustrated and experimentally verified [2].

Acknowledgment
This work is supported by the National Synchrotron Light Source II, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Brookhaven National Laboratory under Contract No. DE-SC0012704 and by New York State Energy Research & Development Authority (NYSERDA).

We thank John Trunk, Eric Dooryhee, Sanjit Ghose, Milinda Abeykoon, Jianming Bai, Danial Olds, Lonny Berman, Steven Hulbert, Gihan Kwon, Wah-Keat Lee, and Peter Siddons (all from Brookhaven Lab) for inspirations and technical assistance We are grateful to Dean Chapman, William Thomlinson, and Tomasz Wysokinski (Canadian Light Source), Xianbo Shi (Advanced Photon Source), Ke Yang (ShangHai Light Source), Ralf Menk and Fulvia Arfelli (Trieste), and Daniel Hausermann (Australian Synchrotron) for helpful discussions about this work. We would like to thank the team at FMB-Oxford, particularly Nigel Boulding who undertook many design calculations for the HEX Laue monochromator. We would like to thank Jennifer Zhong for editorial help.

References:

1 Z. Zhong, D. Bennett, et al, *Synchrotron Radiation News*, **21(3)** (2008) 11-16.

2 Z. Zhong, W. Thomlinson, et al, *Nucl. Inst. Meth. Phys. Res. A.* **450** (2000) 556-567.

3 A.Dilmanian, Z. Zhong, et al, *Phys. Med. Bio*. **45** (2000) 933-946.

4 D. Chapman, W. Thomlinson, et al, *Phys Med. Bio.* **42** (1997), 2015-2025.

5 A. Bravin, P. Coan, & P. Suortti, P. *Phys Med. Bio.* **58** (2013), R1-35.

6 L. Rigon, F. Arfelli, & R. Menk, (2007), *European J. Radiolog*y **68** (2007) S3-S7

7 Y. Zhao, E. Brun, *et al, Proc. Nat. Acad. Sci. USA* **109** (2012), 18290-18294.

8 T. Wysokinski, J. Ianowski, et al, *Phys Med* **32** (2016), 1753-1758.

9 Z. Zhong, M. Hasnah et al, *J. Synchrotron Radiation*, **26** (2019) 1917-1923.

10 Authier, A. (2012). *Acta Crystallogr A* **68**, 40-56.

11 J. Guigay, C. Ferrero, et al, *Acta Crystallogr A* **69** (2013), 91-97.