Development of a Novel Tunable X-Ray Source for the RPI-LINAC

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ABSTRACT

This document summarizes the results of a three year effort to develop a parametric x-ray (PXR) source. The emphasis of this research was to demonstrate production of high yield monoenergetic x-rays. Production of PXR is accomplished by placing a crystal in a relativistic electron beam. The process was first demonstrated in 1985 in Russia. Numerous papers were written about the characteristics of PXR from both experimental and theoretical perspectives. The advantage of PXR over other monoenergetic x-ray sources is that it is produced at large angle relative to the electron beam and at high intensity. None of the previous work described in the literature capitalized on this effect to study what is required in order to generate an effective monoenergetic x-ray source that can be used for practical applications. The work summarized here describes the process done in order to optimize the PXR production process by selecting an appropriate crystal and the optimal conditions. The research focused on production of 18 keV x-rays which are suitable for mammography; however the results are not limited to this application or energy range. We are the first group to demonstrate x-ray imaging using PXR. Such sources can improve current medical imaging modalities. More research is required in order to design a prototype of a compact source.

OUTLINE

The main body of the report is a PhD thesis produced by Bryndol Sones. The thesis contains a detailed description of the work done and the results accomplished.

A list of publications generated in the course of this work is also included.

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**Production of intense, tunable, quasi-monochromatic
X-rays using the RPI linear accelerator**

By
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ABSTRACT

This research investigated the production of parametric X-rays (PXR) using the 60-MeV electron linear accelerator at Rensselaer Polytechnic Institute. PXR is an intense, energy tunable, and polarized X-ray source derived from the interaction of relativistic electrons and the periodic structure of crystal materials. In this work, PXR photon yields and the associated bremsstrahlung background were characterized for graphite, LiF, Si, Ge, Cu, and W target crystals. A model that considers the experimental geometry and crystal mosaicity was employed to predict PXR energy broadening. Measured energy linewidths consistently agreed with predicted values except in cases using poor quality graphite in which the mosaicity was greater than the PXR characteristic angle, 8.5 mrad for 60 MeV electrons. When the predicted energy linewidth was more narrow than our Si X-ray detector resolution, a near-absorption edge transmission technique was used to measure the PXR energy linewidth for Si(400) FWHM of 134 eV at 9.0 keV (2%) and Si(220) FWHM of 540 eV at 17.7 keV (3%).

An experimental study was conducted to select PXR target crystals most appropriate for X-ray production at typical mammography energies (17-20 keV). Low Z materials like graphite and LiF were most suitable for PXR production because of their low Bremsstrahlung production, electron scattering, and photon absorption. Graphite was most efficient at producing PXR photons while the LiF energy linewidth was narrower.

A theoretical model that considers electron multiple scattering, electron divergence, and crystal mosaicity was used to broaden the PXR photon distribution in order to calculate predicted PXR photon yield. This approach, proposed by A.P. Potylitsin, was allowed comparison of measured and predicted PXR yields. The relative error was typically below 0.5. In some cases with LiF, the differences between predicted and measured values were as low as 2% for LiF(400) and 13% for LiF(220). Finally, this work reports for the first time PXR imaging. This was achieved using LiF(220) interacting with 56 MeV electrons with electron beam currents up to 6 μ A.

CHAPTER 1

INTRODUCTION

1.1 Development of Parametric X-rays

M.L. Ter-Mikaelian first proposed the interaction phenomenon for Parametric X-rays (PXR) in his book *High-Energy Electromagnetic Process in Condensed Media* published in 1970 [1]. Referred there as "resonance radiation," PXR is generated from the interaction of relativistic electrons with the periodic structure of single crystals. A broad energy distribution of "virtual photon" is associated with electrons moving through a medium at relativistic speeds. These virtual photons diffract from crystal planes in the same manner that real photons diffract. Bragg's Law governs X-ray diffraction conditions, which relates photon energy, d-spacing between crystal planes, and the incident angle between the photons and the diffraction plane. Consequently, continuously tunable PXR production is possible with the rotation of the target crystal. The first experimental realization of PXR occurred in 1985 [2]. V. G. Baryshevsky used 900 MeV electrons from the Tomsk synchrotron to produce 6.96 keV PXR from the diamond (220) plane. Since then, there have been numerous studies to characterize PXR from silicon (Si) as well as other material like germanium (Ge), highly oriented pyrolytic graphite (HOPG), and tungsten (W) [3,4,5]. From these earlier works, PXR is well known as an intense, directional, tunable, quasi-monochromatic, and polarized X-ray source [6]. In the early 1990s, the dynamical theory of X-ray diffraction was applied by A. Caticha to fully characterize the PXR wave mechanics [7], and this work remains a leading reference in dynamical theory. Another more simplified approach for analyzing PXR is the kinematical theory, which has been validated experimentally [8]. This approach for X-ray diffraction avoids the analysis of a dispersion surface and two wave interference by simplifying the diffraction interaction as a resonance effect as Ter-Mikaelian first proposed. The theory used in this work is kinematical.

In Table 1, X-rays produced from PXR are compared with those from a traditional mammography X-ray machine. For the comparison, the mean X-ray energy is 17.5 keV, and the detection is 50 cm from the source in vacuum. PXR production is calculated from theory with the following assumptions: 60 MeV electrons, 500 μm thick silicon

(220) crystal, 17.5 keV PXR. The X-ray machine production is simulated with Monte-Carlo techniques [9]. Assumptions about the geometry are based on a typical mammography X-ray machine with the following parameters: 30 keV electrons, molybdenum anode at 15° to electron, a molybdenum filter, and detection at 95° from the electron beam [10].

Table 1. Comparison of PXR and X-ray machine X-ray qualities.

<i>Quality</i>	<i>PXR</i>	<i>X-ray Machine</i>
Energy Tunability	Continuous	None
Polarized	Yes	No
Directionality	$1/\gamma \sim 8.5$ mrad	*262 mrad
Limit on Energy Width	Photon Lifetime	K_α Transition
Yield, [Photon/e/cm ²]	2×10^{-6}	3×10^{-8}

*Typical emission fan from anode is 15° .

Traditional X-ray machines use a relatively large electron flux (mA, milli-Amperes) of accelerated electrons with energies in the keV range to produce bremsstrahlung and characteristic fluorescence X-rays in the target anode. Table 1 highlights the distinction between X-rays produced from PXR and those made with the traditional X-ray machine. Most notable, PXR is emitted in a relatively small angular distribution with higher photon production efficiency. The limit on the energy width for both X-ray sources is inherently narrow. PXR energy bandwidth is limited by the inverse photon lifetime, reported in the literature as small as 10^{-3} eV [11]. The atomic K_α transition is a discrete energy, with similarly narrow linewidth. In practice, PXR energy linewidth (FWHM) is highly dependent on the detection collimation. But the continuous bremsstrahlung spectrum from the target anode accompanies the X-ray machine's narrow K_α emission [12]. Figures 1 and 2 show measured spectra from the two sources. The X-ray machine has a large background, while the PXR spectrum is relatively free of background photons.

Figure 1 - Log and linear plots of measured mammography X-ray machine spectrum. Molybdenum anode with molybdenum filter measured with Amptek CdTe X-ray detector.

Figure 2 - Measured PXR spectrum from LiF (220) with Bragg angle of 15° .

1.2 PXR Applications

The uses for PXR rest with the unique characteristics that distinguish PXR from output from the traditional X-ray machine: energy tunability, polarization, directionality, narrow

energy bandwidth with minimal background, and high photon yield. Each PXR application takes advantage of one or more of these PXR characteristics and generally cannot be done easily with traditional X-ray machines.

1.2.1 Optimal X-ray Energy for Medical Imaging.

For medical imaging applications, the traditional X-ray tube, although ubiquitous in hospitals, produces a polychromatic output that can deliver high dose and suffer from significant scattering as the X-rays penetrate tissue [13]. Development of a compact, intense, tunable, narrow bandwidth X-ray source can "open new doors in diagnostic imaging, therapeutics, and biomedical research" [13]. To this end, Kaplin *et al.* have generated PXR by recycling the 33 MeV electrons of a betatron through target materials such as Si, graphite and thin multiplayer films of W and B₄C [14]. PXR has particular potential in resolving the problems with high false-negative and high false-positive rates associated with conventional mammography systems. PXR improves image contrast and reduces dose to the patient because its energy tunability allows delivery of an optimal photon energy for a given breast thickness and composition [15].

1.2.2 K-edge imaging with an injected contrast agent.

At the K absorption edge of a material, there exists a dramatic change in the material's photo-electric linear attenuation coefficient, μ_{PE} . The dominant photon interaction at energies near a material's edge energy is the photon electric effect. In this energy region, the X-ray transmission coefficient through a homogeneous thin sample with thickness x is determined by $e^{-\mu_{PE}x}$. A large change in the transmission through the sample occurs between X-ray energies slightly below and slightly above the K-edge energy. This enhancement of image contrast is achieved with the injection or ingestion of a contrast agent such as iodine or barium in medical imaging techniques [10]. At the iodine K _{α} -edge (33.2 keV) and at the barium K _{α} -edge (37.4 keV), the linear attenuation coefficients jump by factors of 7 and 5, respectively [16]. The image contrast is reduced when using polychromatic output from an X-ray machine. To overcome this complication, others have used synchrotron radiation sources with multiple monochromators as X-ray sources in K-edge digital imaging [17] and in real-time

subtractive angiography (heart imaging) using the iodine tracer [18]. Needing no monochromators, PXR can be efficiently used in K-edge because of its narrow bandwidth and energy tunability about the edge energy.

1.2.3 Material Detection and Identification.

In the K-edge imaging scheme, spatial information from a known tracer material is used to generate medical images. The same principles can be used with a tunable X-ray source to extract information about an unknown absorber. All materials, whether homogeneous or heterogeneous, have a unique attenuation signature determined by its atomic constituents. A tunable, X-ray source can be used as a material probe to either detect or identify an unknown material. This can have applications in security screening for materials such as plastic explosives or uranium. For example, uranium has a K_{α} -edge at 116 keV and L_{α} -edge at 17.1 keV. While the 17.1 keV may not have the penetration depth for security screening, the edge at 116 keV has been proposed in the former Soviet Union using a tungsten crystal.

1.2.4 Phased Imaging Applications.

Phased imaging makes use of distinctions in the real part of a material's index of refraction. The imaginary part of the index of refraction is associated with photon absorption which is the mechanism used for traditional X-ray imaging. However, at the lower X-ray energies currently used for mammography imaging (15-25 keV), phase contrast is about 1000 times more sensitive than traditional absorption contrast imaging [19]. There are three phased imaging configurations: X-ray interferometry, diffraction enhanced imaging, and phase contrast imaging. Each uses of the elastic scattering (refraction) caused from the interaction with the target material and in different ways reconstructs refractive information to form an image of the target. Each demands an intense, monochromatic X-ray source. Recently, synchrotron radiation sources with multiple monochromators have been used to provide sufficient resolution and contrast to in image small objects such as insects in real-time [20, 21, 22]. With current mammography techniques, imaging the human breast is plagued with high false-positive (10%) and false-negative (10-20%) rates, but the composition of the breast has a unique

phase signature that allows distinguishing healthy from cancerous tissue with the use of elastic scattering [23]. PXR is an intense, monochromatic X-ray source that has the potential to be used in elastic scattering experiments.

1.3 Motivation for this work

In each of the applications listed above, an intense, tunable, polarized, or quasi-monochromatic X-ray source is an enabling factor. Nonetheless, the application of PXR to these uses has been only theoretical to this point. PXR has been proposed for medical imaging, but not yet achieved. A PXR facility to calibrate X-ray telescopes has been designed, but not yet built. The aim of this work is to start where the theorist ended and to engineer a useful X-ray source for possible use in the applications discussed above. In achieving this goal, three objective exist:

- Produce tunable X-rays with a narrow energy linewidth (FWHM)
- Produce X-rays with intensity sufficient to image objects with an X-ray CCD camera in a reasonable amount of time
- Minimize background photons (noise)

1.4 Organization of this thesis

This thesis is organized into five chapters. Chapter 1 introduced PXR with a historical perspective and summary of current research status; discussed five possible areas of PXR applications; and established the motivation for this work. Chapter 2 is intended as a comprehensive theoretical resource for designing and executing PXR experiments. Chapter 3 presents the components of the PXR experiments at Rensselaer's Gaertner LINAC Laboratory to include the electron source, the target crystals, and the detection systems. Chapter 4 presents the results from the PXR experiments and includes supplemental theoretical calculations that account for all experimental parameters. And Chapter 5 is an assessment of the PXR results, a compilation of the significance of this work, an evaluation of the achievement this study's objectives, and a proposal for future PXR work at the Gaertner LINAC Laboratory.

CHAPTER 2

THEORY

Parametric X-ray theory bridges across a number of different physical disciplines including: material science, quantum electro-dynamics (QED), X-ray optics, nuclear and particle physics, radiation transport, and radiation detection. This theory is intended to describe all concepts needed to design and execute a PXR experiment with the use of any relativistic electron beam source. To this end, the review of some fundamental concepts is included with hopes of producing a complete, stand-alone theoretical resource for planning, executing, and analyzing future PXR research.

The theory is presented in three sections. The first two sections have an introductory nature necessary to understanding photon and electron interactions related to PXR. In the first section, crystallography covers the structure and nomenclature of PXR target crystals and how real X-rays diffract from these crystals. The second section examines the interaction of relativistic electrons with materials and leads to the specific interactions with periodic structures that produce X-rays. The third section is the much more lengthy topic of PXR production.

2.1 CRYSTALOGRAPHY

The crystallography section is presented in five subsections. The first two are intended to introduce the periodic structure of crystalline material by discussing the Bravais lattice and the crystalline unit cell as a building block of some uniquely arrayed atoms. The next section identifies the repeated planes formed by rows of atoms and defines the terminology of discussing crystallographic planes using Miller indices. The last two subsections explain Bragg's law as the condition that satisfies X-ray diffraction and analyze the intensity of diffraction as a result of the target material (atomic scattering factor) and diffraction plane (form factor).

2.1.1 Bravais Lattice Categories

The growth of a perfect crystal can be visualized as the stacking of an elementary arrangement of atoms called the unit cell. These unit cells are characterized into fourteen

space (Bravais) lattice categories depending on their shape and relative location of atoms in the lattice. Figure 3 shows the different Bravais lattices where circles represent location of atoms and lines represent atomic bonds [24]. The P, I, C, F labels refer respectively, to primitive (P), the German word INNENZENTRIERT (I) referring to body center, the side/plane with centered atom (C), and (F) for all faces centered with an atom.

Figure 3 - The fourteen Bravais lattice unit cells.

For the cubic Bravais lattice unit cells, three basis vectors can define their shape and atom positions; the basis vectors are orthogonal. For the trigonal four basis vectors define the shape and the atom location, three are 120° apart and rest in the trigonal plane (hexagonal

face) and the other is normal to that surface. The silicon or diamond-like unit cell will be used to discuss the Miller Indices that define a diffraction plane, the crystal's reciprocal lattice vector, and the structure factor. Figure 4 shows two perspectives of the silicon unit cell. At the left is the view from any face of this four-fold symmetric unit cell. Vectors **a**, **b**, **c** are the three orthogonal basis vectors, and in the case of the cubic unit cell, each side is the same length, $a=b=c$. For all cubic unit cell, the dimensions $a=b=c$ are subsequently referred to as d_0 , the unit cell dimension. At the right is the 3-D view showing the atom locations in the unit cell volume. A total of 18 atoms are associated with any given silicon unit cell. Atoms at the corners (8) are shared amongst seven other unit cells; atoms at the faces (6) are shared amongst the adjacent unit cells, and atoms in the interior (4) reside solely in the unit cell providing a silicon net atom density of 8 per unit cell volume of d_0^3 .

Figure 4 - Silicon FCC unit cell with basis vectors **a**, **b**, **c**. Shown at right is the 3-D perspective and at left is the view of any of the six faces.

2.1.2 Unit Cell Dimensions

In the PXR experiments, we are primarily concerned with three types of crystal unit cells: face centered cubic (FCC) such as silicon, lithium fluoride, germanium, and diamond; hexagonal such as highly oriented pyrolytic graphite (HOPG); and body centered cubic (BCC) such as tungsten and beryllium. These three different structures provide uniquely different characteristics for X-ray diffraction and PXR production. What follows is a discussion of the unit cell, Miller indices, the reciprocal lattice vector, Bragg's Law for X-ray diffraction, form factors and structure factors, and conditions for

forbidden X-ray reflections. Where examples are needed, the silicon crystal is used for discussion.

Table 2 summarizes the unit cell parameters for these crystals. Z (atomic number) is the number of electrons per atom; in the case of the compound LiF, Z is the effective charge. The net number of atoms per unit cell is listed as well as the unit cell dimension d_0 for the cubic unit cell, and d_0 and c , which is the longer dimension of the hexagonal unit cell of graphite.

Table 2. Summary of crystal unit cell dimensions.

Crystal	Z	# of Atoms	Dimension [$\text{\AA}$]
Beryllium (Be)	4	2	$d_0=2.286$ $c=3.583$
Graphite (HOPG)	6	4	$d_0=2.461$ $c=6.708$
Diamond (C)	6	8	$d_0=3.567$
Lithium Fluoride (LiF)	8.31	4	$d_0=4.026$
Silicon (Si)	14	8	$d_0=5.431$
Copper (Cu)	29	4	$d_0=3.615$
Germanium (Ge)	32	8	$d_0=5.658$
Tungsten (W)	74	2	$d_0=3.165$

2.1.3 Crystallographic Planes and Miller Indices

The arrangement of multiple unit cells can be used to visualize the periodic structure of atoms in the crystal material. Figure 5 shows the arrangement of several silicon unit cells from the perspective of the basis vector $\mathbf{a}$, $\langle 100 \rangle$, coming out of the page. The plane of the page is formed by the basis vectors $\mathbf{b}$ and $\mathbf{c}$. Not draw to scale, a silicon wafer is superimposed on Figure 5 to demonstrate a common wafer manufacturing nomenclature. In this case, the wafer has a surface of (100) with an orientation flat in the vector direction $\langle 011 \rangle$. The flat is the linear portion cut into the circular shaped wafer. The darkened, equally spaced diagonal lines of silicon atoms represent the silicon (022) family of crystallographic planes. The three numbers used in the descriptions above are called the Miller Indices, h , k , and l . Numbers in brackets $\langle hkl \rangle$ refer to a vector. The

h, k, l indices corresponding to the unit vector coordinates in the unit cell basis vectors **a**, **b**, **c**, respectively. Numbers in parenthesis (hkl) refer to the family of parallel planes perpendicular to the vector $\langle hkl \rangle$. For example, in Figure 5 the wafer surface (100) is normal to basis vector **a**, $\langle 100 \rangle$. For the trigonal unit cells like graphite, four Miller Indices are used h, k, i , and l where h, k , and i correspond to the basis vectors in the hexagonal face and l corresponds to the basis vector normal to that face.

Figure 5 - View of the silicon unit from the $\langle 100 \rangle$ direction. Silicon wafer superimposed to show (100) surface and $\langle 011 \rangle$ orientation flat.

For X-ray analysis in phase space, it is far more convenient to examine the crystal family of planes using a vector notation for the normal to the plane and the reciprocal space for the distance between planes. The reciprocal lattice vector, $\vec{\tau}$, is a vector with direction normal to a crystallographic plane and with magnitude inversely proportional to the "d-spacing" distance between the planes. In

Figure 6, two silicon unit cells are shown with the Si (220) plane highlighted in the one on the left, and the Si (111) plane highlighted in the other. The direction of $\vec{\tau}$ in these two examples is perpendicular to the planes, and parallel to the vectors $\langle 220 \rangle$ and $\langle 111 \rangle$, respectively. The hkl can be used to easily draw the planes using the fact that the intersection of the plane with any of the basis vectors, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ is the inverse of the corresponding h, k, l . The Si (220) plane intersects the basis vectors at $d_o^*(1/2, 1/2, 0)$, where d_o is the unit cell dimension. For simplicity, the dimension of the cubic unit cell will be subsequently referred as d_o and the distance between (hkl) planes is d_{hkl} . The distance between planes in a cubic unit cell relates to the unit cell dimension, d_o , and (hkl) through the following relationship.

$$d_{hkl} = \frac{d_o}{\sqrt{h^2 + k^2 + l^2}} \quad (1)$$

The magnitude of $\vec{\tau}$ is inversely related to d_{hkl} , and is defined below in phase space for the cubic unit cell.

$$|\vec{\tau}| = \frac{2\pi}{d_{hkl}} = \frac{2\pi}{d_o} \sqrt{h^2 + k^2 + l^2} \quad (2)$$

Figure 6 - Silicon FCC unit cell with basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. Diffraction planes for (h, k, l) Miller Indices (220) at left and (111) at right.

2.1.4 Bragg's Law for X-ray Diffraction

Bragg's law governs the diffraction of X-rays from a given crystallographic plane. In vector form, Bragg's law relates the X-ray's initial wave vector $\vec{k}_i$, final wave vector $\vec{k}_f$, and the reciprocal lattice vector $\vec{\tau}$.

$$\vec{k}_f - \vec{k}_i = \vec{\tau} \quad (3)$$

A physical interpretation of this elastic scattering process can be viewed in phase space through the use of the Ewald sphere. At its center, the sphere portrays the point-like interaction of an X-ray with a crystal plane. The radius of the sphere is inversely related to the wavelength of the X-ray (λ), $\text{radius} = |\vec{k}_f| = |\vec{k}_i| = \frac{2\pi}{\lambda}$. In Figure 7, the Ewald sphere is superimposed with a crystal with some arbitrary crystal plane. The incident X-ray forms an angle with the crystal plane, θ_B , called the Bragg angle. The diffracted X-ray scatters from its original direction by $2\theta_B$.

Figure 7- Ewald sphere representation of X-ray diffraction, governed by Bragg's Law.

In scalar form, Bragg's Law is interpreted from Equation 2 to form conditions allowing diffraction. Diffraction depends on the photon incident angle (θ_B) made with the plane, any integer multiple (m) of the wavelength (λ), and the distance (d_{hkl}) between planes.

$$2d_{hkl} \sin(\theta_B) = m\lambda \quad (4)$$

2.1.5 INTENSITY OF DIFFRACTION: ATOMIC SCATTERING AND FORM FACTORS

Although Bragg's law in either vector or scalar form defines the necessary conditions for X-ray diffraction, there still remains further study of the entire scattering process to examine the extent of diffraction that will occur. Two additional quantities are introduced: the atomic scattering factor (f) relates to the photon scattering from a single atom, and the form factor (F_{hkl}) relates the photon scattering from the ensemble of atoms in the crystal's unit cell. The atomic scattering factor is the ratio of the amplitude scattered by the atom to the amplitude scattered by a single electron of the atom. Consequently, the maximum value for f for any given element is its atomic number, Z . This condition is at a scattering angle of 0° when the scattered X-rays are all in phase. As the scattering angle increases, the scattering amplitude decreases as a result of larger phase differences between scattered X-rays. Plots of the atomic scattering factor are typically made as a function of momentum transfer $s = \sin(\theta)/\lambda$, where θ is the incident angle. An analytical expression can be used with the empirically measured Cromer-Mann coefficients a_i , b_i , c for $i=1-4$ to calculate the atomic scattering factor [25]. The coefficients are atom dependent, and the model is valid up to $s=2 \times 10^{-10} \text{ m}^{-1}$.

$$f(s) = c + \sum_{i=1}^4 [a_i (\exp(-b_i k^2))] \quad (5)$$

Figure 8- Calculated atomic scattering factor for silicon, $Z=14$ using Equation 5.

From Equation 4, $\sin\theta/\lambda=1/(2d_{hkl})$ so that the atomic scattering factor $f(s=1/(2d_{hkl}))$ can also be interpreted as a function of (hkl) when the Bragg condition is satisfied. Also shown in Figure 8 are the s values for the Si (111) and Si (220) planes with their corresponding atomic scattering factors. Si (111) with its larger d -spacing and lower Miller indices has the larger atomic scattering factor compared to Si (220).

The atomic scattering factor is used to calculate the form factor for a given (hkl) plane in a unit cell. The form factor determines the level of interference from the different scattering atoms in the unit cell. As with any wave interference, the wave amplitude from the different scattering atoms in the unit cell can sum constructively to produce a larger amplitude or sum destructively to produce an amplitude of zero. The later case is the extinction condition or forbidden reflection for which no diffraction intensity occurs. The form factor is calculated below for a given (hkl) [26]. N is the net number of atoms in the unit cell; f is the atomic scattering factor; u_n , v_n , w_n are the fractional coordinates of the n th atom in the unit cell corresponding to the **a**, **b**, **c** basis vectors, respectively.

$$F_{hkl} = \sum_{n=1}^N f_n \exp[2\pi i(hu_n + kv_n + lw_n)] \quad (6)$$

As an example, Table 3 shows the fractional coordinates of the eight atoms in the silicon unit cell. For silicon, $N=8$ and f_n for all eight atoms is the silicon atomic scattering factor for the appropriate (hkl). For any single element crystal, f_n can be taken out of the summation in Equation 6 leaving the summation of the exponential terms. This term is often called the structure factor, S_{hkl} .

$$S_{hkl} = \sum_{n=1}^N \exp[2\pi i(hu_n + kv_n + lw_n)] \quad (7)$$

Table 3. Fractional unit cell locations for the eight Si atoms.

u	v	w
0	0	0
0	1/2	1/2
1/2	0	1/2
1/2	1/2	0
1/4	1/4	1/4
1/4	3/4	3/4
3/4	1/4	3/4
3/4	3/4	1/4

The intensity of the diffracted X-ray is proportional to the wave amplitude squared. Consequently, the intensity for X-ray diffraction can be calculated as the square of the atomic scattering factor, $f(k)$, times the square of the structure factor, S_{hkl} . S_{hkl}^2 for all (hkl) takes the values 64 for all even (hkl), 32 for all odd (hkl), or 0 for other (hkl) combinations. The (hkl) planes providing the value of zero satisfy the extinction condition, and the reflections from these (hkl) planes are considered forbidden. For similar reasons, other types of unit cells have conditions for diffraction extinction, and general rules have been established for identifying forbidden reflections. Rules for forbidden reflections are shown in Table 4.

Table 4. Rules for forbidden reflections.

Unit Cell	Forbidden Reflection	Examples
FCC	hkl have different parity	(100) (121)
BCC	hkl sum to odd number	(111) (220)
Hexagonal	l is odd	(0001) (0003)

2.2 RELATIVISTIC ELECTRON INTERACTION WITH MATTER

The electron interaction section is presented in four subsections. As electrons interacts with a material, collision and radiation losses occur depositing heat and generating photons in the material. The electrons also scatter from the interaction with the material. The first three subsections discuss the mechanics of these three effects. When examples are necessary, four materials with representative crystal thickness are compared: graphite (1 mm), lithium fluoride (1.5 mm), silicon (0.5 mm), and tungsten (1 mm). The last subsection also discusses some novel X-ray sources derived from the interactions of relativistic electrons with periodic structures.

2.2.1 Electron Heat Deposition.

Electron collisions produce heat in the target material. The collision energy loss is proportional to the atomic number, Z , of the target material. The rate of energy loss, dE , per unit distance, dx , can be calculated using the expression below [28]. e is the fundamental unit charge, N is the target number density, and m_e and v are the rest mass and velocity of the electron. B is a parameter dependent on the ionization energy, I , of the target material and the velocity of the incident electron, $\beta=v/c$.

$$-\left(\frac{dE}{dx}\right)_c = \frac{2\pi e^4 N Z}{m_e v} B \quad (8)$$

$$B = \ln\left(\frac{m_e v^2 E}{2I^2(1-\beta^2)}\right) - \ln 2 \left(2\sqrt{1-\beta^2} - 1 + \beta^2\right) + (1-\beta^2) + \frac{I}{8} \left(1 - \sqrt{1-\beta^2}\right)^2 \quad (9)$$

The stopping power for most materials is well tabulated and easily found at National Laboratory or National Institute for Standards and Technology (NIST) databases. Below is a table showing a few materials with their atomic number, the output from the NIST

Estar Data Base [27] for 60 MeV incident electrons, and the calculated power deposition per μA of electron beam current per cm of target material thickness.

Table 5. Electron power deposition through collision losses in various crystal materials.

Crystal	Atomic Number Z	Collision Energy Deposition [MeV*cm ² /g]	Density [g/cm ³]	Power Deposition [W/ μA /cm]
Graphite	6	1.91	1.70	3.2
LiF	8.3	1.74	2.64	4.6
Si	14	1.87	2.33	4.4
W	74	1.38	19.30	26.6

Note from Table 5, the tungsten Z is about five times greater than the silicon Z and power deposition scales appropriately to changes in Z.

2.2.2 Bremsstrahlung Production.

Radiation energy losses compete with collision energy losses. In general, low energy electron interactions are dominated by collision losses. But as the electron increases in energy the radiation energy losses become more dominant. Figure 9 shows the electron collision and radiation stopping powers for silicon as a function of electron energy. At the electron energy of 1 MeV, radiation energy losses start to grow exponentially with increasing electron energy and become dominant in silicon above 52 MeV.

Figure 9- Graphs of collision and radiation stopping power losses for electrons interacting with silicon.

An empirical expression for estimating the ratio of radiation to collision stopping power is shown below [28], where E is the electron energy in MeV and Z is the atomic number.

$$\frac{\left(\frac{dE}{dx}\right)_R}{\left(\frac{dE}{dx}\right)_c} \approx \frac{EZ}{700} \quad (10)$$

The radiation losses occur from coulomb interactions causing a deceleration of the electrons and the emission of bremsstrahlung radiation. Unlike the collision losses, the bremsstrahlung yield increases with Z^2 rather than Z . For relativistic electrons, the bremsstrahlung is directional, emitted in the forward direction in a cone with solid angle of about γ^{-1} , where γ is the Lorentz Factor, $\gamma=E/(m_0c^2)$. For 60 MeV electrons, the bremsstrahlung cone makes an angle of about 0.5 degrees with the electron initial direction.

A precise calculation for the bremsstrahlung photon yield can be made with an analytical expression for production per unit length and with consideration of photon absorption along the target escape route. The expression below calculates the bremsstrahlung production, N_{BS} , for a given target material, photon frequency ω , electron

energy E_e , and angle θ from the electron direction [29]. N is the number density of the target, and r_o is the classical electron radius.

$$N_{BS} = N \frac{8}{137\pi\omega} Z^2 r_o^2 \gamma^2 \left(\frac{233}{Z^{1/3}} \right) \left[\frac{1 + \gamma^4 \theta^4}{(1 + \gamma^2 \theta^2)^4} \right] \quad (11)$$

The term in brackets defines the angular distribution of bremsstrahlung photons from the path of the incident electrons. For 60 MeV electrons, $\gamma^{-1}=8.5$ mrad at which the intensity drops to 12.5%. Most of the bremsstrahlung photons are emitted in the γ^{-1} solid angle. Higher electron energies confine the bremsstrahlung to a smaller angular distribution. This is demonstrated in Figure 10 where the term in brackets is plotted as a function of θ for different electron energies.

Figure 10- Bremsstrahlung angular distribution shown for electron energies: 30, 60, 120, 240, and 480 MeV.

The bremsstrahlung production in Equation 11 is the number of quanta per electron per unit electron track length in the material. Once produced, photon absorption must be considered along the photon escape pathway in the material. This is a geometric consideration determined for a specific bremsstrahlung energy and emission angle.

2.2.3 Electron Scattering

To this point, the dynamics of the electron-material interaction has focused on the products left in the target material. The interaction also affects the electron momentum. The electrons lose energy in the material. Consider the example crystals again. Table 6 below shows the calculated energy loss for 60 MeV electrons in a range of target crystals with representative thickness [27]. With exception to tungsten in which 60 MeV electrons lose approximately 30% of their incident energy, the other low Z crystals have minimal effect on the incident electron energy.

Table 6. Total energy loss from electron interactions with representative crystal thickness.

Crystal	Total Energy Loss [MeV*cm ² /g]	Thickness [mm]	Fractional Energy Loss
Graphite	3.09	1	8.7 x 10 ⁻³
Lithium Fluoride	3.04	1.5	2.0 x 10 ⁻²
Silicon	4.24	0.5	8.2 x 10 ⁻³
Tungsten	9.25	1	3.0 x 10 ⁻¹

The electron multiple scattering in the material is the next consideration. An analytical expression is used to estimate the gaussian standard deviation, σ_{ms} , of the electron scattering angle distribution. This is only valid for thin samples of a few radiation lengths, X_o . For an energetic charged particle passing through a medium, the radiation length is the traveled distance at which the particle energy is reduced by radiative losses to e^{-1} (~36.8 %) of its incident energy [30]. The X_o can be calculated below as a function of the target material density ρ , atomic number Z , and atomic mass A [11].

$$X_o = \frac{(716.4)A}{\rho Z(Z+1) \ln\left(\frac{287}{\sqrt{Z}}\right)} \quad (12)$$

With the radiation length determined, the standard deviation of the electron scattering angle, σ_{ms} , in radians can be calculated using the following analytical expression [11]. E_e is the electron energy in MeV, and d is the material thickness in cm.

$$\sigma_{ms} = \frac{13.6}{E_e} \sqrt{\frac{d}{X_o}} \left(1 + 0.038 \ln\left(\frac{d}{X_o}\right) \right) \quad (13)$$

The approach for calculating the radiation length presumes that the electrons have energy greater than 1 GeV such that the radiative energy loss dominates the collision energy loss $dE/dx_{rad} \gg dE/dx_{col}$. At 1 GeV, the ratio of radiative to collision linear energy loss in silicon is 21.2 [27]. With the use of 60 MeV electrons, radiative losses do not dominate. Using Equation 10, the ratio of radiative to collision linear energy loss is just 0.5 for graphite and 6.3 for tungsten. A modified approach to using the radiation length X_o in Equation 13 is to use the traveled distance, X , at which the particle energy is reduced by total losses (radiative and collision) to e^{-1} of its incident energy. The traveled distance, X , is subsequently referred as the *interaction length*. X can be determined from the electron energy (E_e), the material density (ρ) and the tabulated total stopping power (S) with units $[(MeV \cdot cm^2)/g]$ [27] for that electron energy using the expression below.

$$X = \frac{E_e}{S\rho} \quad (14)$$

X may be more appropriate for use in calculating σ_{ms} in Equation 13. To compare the example crystals, Table 7 shows the material radiation length (X_o), the energy loss length (X), and the calculated standard deviation of the electron scattering angle for the 60 MeV electrons using both lengths; X_o values are shown in parentheses.

Table 7. Total energy loss from 60 MeV electron-crystal interactions.

<i>Crystal</i>	<i>Linear Stopping Power, dE/dx [MeV/cm]</i>	<i>Radiation Length, X_o [cm]</i>	<i>Energy Loss Length, X [cm]</i>	<i>Thickness [mm]</i>	<i>Standard Deviation of Scattering Angle, σ_{ms} [mrad]</i>
Graphite	7.0	16.4	11.4	1	(14) 17
Lithium Fluoride	8.0	12.0	7.5	1.5	(21) 27
Silicon	9.9	9.4	6.1	0.5	(13) 17
Tungsten	178.5	0.35	0.34	1	(115) 118

A first order assessment of the importance of the electron multiple scattering is to compare the standard deviation of the electron scattering angle with the bremsstrahlung distribution angle. Recall that the bremsstrahlung emission angle is approximately γ^{-1} or 8.5 mrad for 60 MeV electrons. In Table 7, the calculated σ_{ms} for graphite, lithium fluoride, and silicon are within a factor of three of the bremsstrahlung emission angle, but in the case of tungsten σ_{ms} is more than a order of magnitude greater. Another consideration is the electron scattering in air. For example, the standard deviation of the electron scattering angle for 60 MeV electrons through 2.54 cm and 25.4 cm air pathways are 1.4 mrad and 5.0 mrad, respectively. Unlike the energy loss as a result of the material interaction, the electron multiple scattering plays an important role in the understanding of radiative processes that occur from the interaction of relativistic electrons and material.

2.2.4 Other Novel X-ray Radiation Sources

There are a number of novel radiative processes that result from interactions involving relativistic electrons. Four involve relativistic electron and dense materiel like crystals: Transition Radiation (TR), Coherent Bremsstrahlung (CB), Channeling Radiation (CHR), and Parametric X-rays (PXR). This section provides a short overview of the mechanism of the first three X-ray sources and then distinguishes them from PXR

2.2.4.1 Transition Radiation

Transition Radiation (TR) occurs when the relativistic electron passes from one medium to another. The perturbation of the electron's electric field when passing from one material dielectric to another generates emission of electromagnetic radiation. As with any electromagnetic wave at an interface, there is a reflected and transmitted component [1]. The most intense emission is in the direction defined by γ^{-1} [6]. TR is polychromatic with frequencies in the optical regime increasing a few orders of magnitude up to approximately $\gamma\omega_p$, where ω_p is the exit material plasma frequency [1]. For example, transition radiation from a 60 MeV electron passing from silicon ($\hbar\omega_p=31$ eV) to vacuum can emit frequencies in the visible regime and X-ray energies up to 3.6 keV. TR has been used in X-ray production with schemes of multi-foil targets, electron beam energy measurements from forward or backward directions, and electron beam

characterization with use of backward optical transition radiation (OTR). Higher energy electrons can produce higher energy X-rays although TR emission remains close to the electron beam direction.

Figure 11- Schematic of forward Transition Radiation (TR) with continuous frequencies emitted in the γ^{-1} cone about the electron trajectory.

2.2.4.2 Coherent Bremsstrahlung

Coherent Bremsstrahlung is a special form of bremsstrahlung in which the electron trajectory is very close to the line of crystal atoms that form a crystallographic plane. The electron trajectory is slightly perturbed through the periodic interaction with the atoms; electrons are attracted towards the atomic rows. The electron periodically crosses the row of atoms allowing a coherent interaction of selected wavelengths in the bremsstrahlung continuous spectrum. Because of this periodic interaction, the intensity of these selected wavelengths is enhanced through constructive interference. The necessary condition for this to occur is that the emitted photon momentum transfer matches the reciprocal lattice vector, $\vec{\tau}$, for a given plane with Miller Index (hkl). As in the Mossbauer Effect, momentum conservation also requires that the entire crystal absorb the atom recoil. For a given electron trajectory, there may be a number of (hkl) that satisfy this condition producing a CB spectrum with peaks at these frequencies. CB emission is generally confined to the γ^{-1} forward direction of the bremsstrahlung cone. While photon energies in the MeV energy range are produced at most high-energy GeV electron accelerators, CB down to several keV has yet to be successfully exploited [6]. In addition to (hkl), the characteristic CB energies also depend on the incident angle to the plane with the upper limit to satisfy the coherence condition related to γ^{-1} down to a lower limit that then confines the electron to the channel between the planes.

Figure 12- Schematic of Coherent Bremsstrahlung (CB) with several enhanced frequencies emitted in the γ^{-1} cone about the electron trajectory.

2.2.4.3 Channeling Radiation

Channeling Radiation (CR) occurs when the electron trajectory is incident along crystal planes and confined to the channel between the planes. The effect is analogous to undulator radiation generated from the electron's interaction with alternating magnetic fields. In the CR case, small angle collisions near the atom row cause electron oscillatory motion due to electron acceleration, which is nearly perpendicular to the direction of propagation. For small incident angles, this transverse acceleration can corresponds to the discrete bound energy levels in the material's transverse potential. The quantum mechanical analogy is made to describe CR emission as the transition between discrete bound states. The material's electric potential well describes the discrete CR emission frequencies, and higher electron energies allow transition from higher bound states and hence satisfying even more allow discrete CR frequencies [6]. Again the emission is in the forward direction defined by γ^{-1} .

Figure 13- Schematic of Channeling Radiation (CR) with discrete material specific frequencies emitted in the γ^{-1} cone about the electron trajectory.

2.2.4.4 Comparison to PXR

This comparison is based on the aim of producing X-rays in the region of a few keV to 100 keV. For that reason, no further discussion of Coherent Bremsstrahlung is made because it is used to produce forward high-energy gamma rays and has yet to be used for energies in our region of interest. The radiative processes of Transition Radiation (TR), Channeling Radiation (CHR) and Parametric X-rays (PXR) are compared. CHR is linearly polarized, and TR and PXR are linearly polarized under certain conditions. Table 8 compares the three sources in terms of energy bandwidth $\Delta\omega/\omega$, the photon distribution angle of the X-ray emission, the feasibility for changing the X-ray energy, and the historically achieved intensity in expressed in units of (photons/s/mrad²/1% bandwidth) under idealized experimental configurations with a hypothetical 100 μ A electron beam current [6].

Table 8. Comparison of Transition Radiation (TR), Channeling Radiation (CHR), and Parametric X-rays (PXR).

<i>Source</i>	<i>Bandwidth</i> $\Delta\omega/\omega$	<i>Emission Direction</i>	<i>Energy Tunability</i>	<i>Emission Cone</i>	<i>Intensity</i> [ph/s/mrad ² /1% bw]
TR	50%	Forward	Not Practical	γ^{-1}	10^8
CHR	10%	Forward	Not Practical	$1/3\gamma^{-1}$	10^8
PXR	1%	$2\theta_B$	Simple	γ^{-1}	10^8

In Table 8, the first notable difference between the three sources is in the energy bandwidth. The PXR bandwidth is far superior providing a quasi-monochromatic X-ray. The emission angle for TR and CHR is constrained to the forward direction along the electron trajectory, while PXR can be generated at large angles to the electron beam. The X-ray energy of each of the sources can be changed with varying degrees of difficulty. The TR energy can be changed by widely varying the electron energy. By selecting different target materials with different electron bound states, the CHR energy can be changed. These changes are not practical for energy tunability. On the other hand, PXR is continuously tunable with only the rotation of the target crystal with respect to the incident electron beam. The photon emission cone defines the angular distribution in

which most of the source photons are emitted. The photon beam apertures for the three sources are generally equal, although CHR has emission of one-third the γ^{-1} emission cone. Finally, TR and CHR produce more photons in the energy bandwidth $\Delta\omega/\omega$ although the three sources intensities are equivalent when adding the 1% energy bandwidth constraint.

2.3 PARAMETRIC X-RAYS

The theoretical discussion of PXR starts with the virtual photon method that correlates the relativistic electron's electric field to the transverse electric field of light propagating in the same direction as the electrons. This is followed by a physical interpretation to the electron periodic perturbation at crystal planes that satisfies resonance conditions analogous to Bragg's Law of Diffraction. Then PXR energy and photon distribution is analyzed using idealized conditions. This section ends with a more detailed study of PXR energy and photon distribution under more realistic experimental conditions.

2.3.1 Virtual Photon (Pseudo Photon) Method

There are conditions in quantum electro-dynamics (QED) in which the electric field of a moving charge particle can be dominated by that component perpendicular to the direction of motion. The method for this approximation results in the charged particle taking the physical characteristics of electromagnetic radiation propagating in the direction of the electron motion. With light, the electric field and magnetic field are always perpendicular to each other and perpendicular to the direction of propagation. However, for a slow moving charged particle this is not the case. In Figure 14 an electron is moving to the right with a speed v , and the electric field at a position r has components parallel to and perpendicular to the electron direction, $E_{\perp}$ and $E_{\parallel}$, respectively. " vt " is the distance traveled in some time t , and ρ is the projection of r in the direction perpendicular to the electron motion.

Figure 14- The drawing of a moving electron and the perpendicular and the parallel components of its electric field.

The magnitude of the parallel and perpendicular components of the electron's electric field can be calculated using the equations below [1]. As v approaches c , the speed of light, the parallel component $E_{||}$ becomes small compared to the perpendicular component $E_{\perp}$. At relativistic speeds the electron's electric field takes the form of a disk-like (pancake) shape in the transverse or perpendicular direction.

$$E_{||} = \gamma \frac{evt}{(\rho^2 + v^2 t^2 \gamma^2)^{3/2}} \quad (15)$$

$$E_{\perp} = \gamma \frac{e\rho}{(\rho^2 + v^2 t^2 \gamma^2)^{3/2}} \quad (16)$$

Two important conclusions can be made from this approach. First, the electron's electric field is effectively perpendicular to the direction of motion, and the conditions similar to the propagation of light are established that validate the virtual photon approach. Second, the numerator of Equation 16 can be evaluated to establish a time/space for which $E_{\perp}$ is largest. At time intervals t_{eff} (defined below), $E_{\perp} = \gamma E_{||}$.

$$t_{eff} \approx \frac{\rho}{v} \sqrt{1 - \beta^2} \quad (17)$$

The electric field is determined to be concentrated at a distance vt_{eff} from the electron in the plane containing the electron and perpendicular to the direction of motion. As the electron's velocity increases, the shape of the electron's electric field is squeezed further in the parallel direction and the disk extends farther in the perpendicular direction. This elongation of $E_{\perp}$ for the particle electron has the effect of a set of photons with various frequencies. The virtual photon field of an electron traversing some material can be interpreted as a broad distribution of photon energies. These virtual photons diffract from crystallographic planes in the same manner that real photons diffract according to Bragg's Law. The result is the emission of real photons that satisfy an appropriate resonance condition.

2.3.2 Resonant Electron Perturbations

Consider a relativistic electron with velocity $\vec{V}$ traversing a family of crystallographic planes defined by the reciprocal lattice vector $\vec{\tau}$ in the geometry shown in Figure 15.

Figure 15- The drawing of a relativistic electron traversing crystallographic planes with photon emission in direction $\hat{\Omega}$.

For any given direction $\hat{\Omega}$, there exists a condition for which constructive interference occurs between the initial and subsequent evenly spaced interactions with the crystallographic planes. To analyze this, the time, Δt , between electron interactions with adjacent atomic rows of the planes is defined in the following manner.

$$\Delta t = \frac{2\pi}{|\vec{\tau} \cdot \vec{V}|} \quad (18)$$

Let the radiation emitted in the direction $\hat{\Omega}$ have wavelength, λ . Then, the radiation will add constructively if the path length difference between radiation emitted from subsequent rows of atoms along the direction $\hat{\Omega}$ is an integer multiple of λ . The condition for this to occur is shown below. The first term represents the distance traveled by the initial emitted radiation and the second term represent the distance travel by the subsequent emitted radiation after time, Δt . n_λ is any integer multiple [31].

$$\frac{c}{\sqrt{\epsilon_0}} \Delta t - \vec{V} \cdot \hat{\Omega} \Delta t = n_\lambda \lambda \quad (19)$$

The virtual photon field provides continuous values for λ , and the situation in Equation 19 is satisfied for all orientations restricted only by the X-ray forbidden reflections shown in Table 4.

2.3.3 Parametric X-ray Energy

The PXR energy is highly dependent on the geometric relationship between the electron velocity, the reciprocal lattice vector, and the PXR detection angle. In this section, the relationship between the PXR energy and these vectors is first discussed. A three dimensional coordinate is established to express the vectors in scalar components. If these three vectors all rest in a single diffraction plane, then a simplification is made to define the PXR energy in two dimensions in which the characteristics of PXR energy are discussed. Finally, a return to the three-dimensional model allows for a more detailed analysis of the energy broadening. The electron beam divergence, electron beam spot size, the detector collimator size, the distance from crystal to the detector, and crystal mosaic spread all affect the PXR energy linewidth.

2.3.3.1 Equation For PXR Energy.

Equation 19 represents the condition in which PXR is generated. The wavelengths that satisfy Equation 19 also define the PXR energy through the relationship $E_{PXR}=hc/\lambda$, where h is Plank's constant. After some algebra, the PXR energy can be calculated using the expression below [31].

$$E_{PXR} = \hbar\omega_{PXR} = n_{\lambda} \frac{c\hbar|\vec{\tau} \cdot \vec{V}|}{c - \sqrt{\epsilon_0} \vec{V} \cdot \hat{\Omega}} \quad (20)$$

Again, c is the speed of light, $\vec{\tau}$ the crystal plane reciprocal lattice vector, $\vec{V}$ the electron velocity vector, n_{λ} an integer multiple of the wavelength, and $\hat{\Omega}$ the unit vector in the direction of PXR emission. ϵ_0 is the crystal permittivity defined below as a function of the material plasma frequency, ω_p .

$$\epsilon_0 = 1 - \frac{(\hbar\omega_p)^2}{(E_{PXR})^2} \quad (21)$$

For nearly all crystals, $\hbar\omega_p \ll E_{PXR}$ for X-ray production, and $\epsilon_0 \sim 1$. Parametric X-rays are a continuously tunable X-ray source. Except for unusual experiments with detection of PXR near the direction of a low energy electron beam (~ 15 MeV), the PXR energy is effectively independent of the incident electron energy and is determined solely by the crystal spacing between planes and the experimental geometry.

2.3.3.2 Three Dimensional Coordinate System

It is often beneficial to use a spherical coordinate system to define the geometry of the PXR production. Figure 16 depicts the vectors $\vec{\tau}$, $\vec{V}$, $\hat{\Omega}$ in the three dimensional X, Y, Z coordinate axes. For convention, the electron velocity is along the X axis, the PXR interaction occurs at the origin, the reciprocal lattice vector $\vec{\tau}$ rests in the X-Y plane and makes the angle ϕ with the positive Y-axis, and the PXR emission angle is defined with the polar angle Ω made with the positive X-axis, and the azimuthal angle, α , made with the X-Y plane in the positive Z direction. θ_x and θ_y represent a new coordinate axes for the PXR detector face centered on $\hat{\Omega}$ and normal to the diffraction plane defined by

the vectors $\vec{\tau}$ and $\vec{V}$. θ_x is an angular displacement from the origin and in the diffraction plane, and θ_y is an angular displacement from the origin and perpendicular to the diffraction plane.

Figure 16- Convention for defining PXR production in scalar component form.

Using the convention of Figure 16, the scalar component-form of the three vectors $\vec{\tau}$, $\vec{V}$, $\hat{\Omega}$ are written below. Unit vectors are shown for simplicity, V_0 represents the initial velocity vector, and subscripts x, y, z correspond to the axes in Figure 16

$$V_{0x} = 1; V_{0y} = 0; V_{0z} = 0 \quad (22)$$

$$\tau_{0x} = -\sin \phi; \tau_{0y} = \cos \phi; \tau_{0z} = 0 \quad (23)$$

$$\Omega_x = \cos \Omega; \Omega_y = \sin \Omega \cos \alpha; \Omega_z = \sin \Omega \sin \alpha \quad (24)$$

2.3.3.3 PXR Energy in the Diffraction Plane

The above component-form for the vectors $\vec{\tau}$, $\vec{V}$, $\hat{\Omega}$ is particularly useful in analyzing the PXR production when experimental parameters such as electron multiple scattering or detector solid angle are considered. For the moment, this rigorous analysis will be held for later so that the fundamental characteristics of PXR production can be studied. In this case, the problem is simplified so that $\vec{\tau}$, $\vec{V}$ and $\hat{\Omega}$ all lie in the X-Y plane ($\alpha=0$). The two dimensional view of vectors $\vec{\tau}$, $\vec{V}$ and $\hat{\Omega}$ are shown in Figure 17. The expression for calculating the PXR energy for a given crystallographic plane with a reciprocal lattice vector $\vec{\tau}$ is shown below [32].

$$E_{PXR} = \hbar\omega_{PXR} = \hbar c \frac{\tau \sin \phi}{1 - \cos \Omega} \quad (25)$$

The electron incident angle (ϕ) is measured with respect to the crystal planes, and the PXR emission angle (Ω) is measured with respect to the electron velocity. Bragg's Law is satisfied for the condition $\Omega=2\phi$ around which produces the maximum PXR intensity.

Figure 17- Two-dimensional view of PXR vectors $\vec{\tau}$, $\vec{V}$ and $\hat{\Omega}$.

For a given crystallographic plane, PXR energy can be tuned by rotating the target crystal or by moving the detector while seeking to preserve the Bragg condition ($\Omega=2\phi$) for greatest PXR intensity. When the Bragg condition is satisfied, Bragg's Law (Equation 4) is consistent with the equation for PXR energy (Equation 25); θ_B and ϕ are then identical. The energy is a function of d-spacing, ϕ , and Ω . Consider some functional relationships to these three parameters that produce greater PXR energy. Planes with smaller d-spacing produce PXR with greater energy, and this can be achieved by using crystals with smaller unit cells or by using planes with higher (hkl). At the Bragg condition,

smaller ϕ produce PXR with greater energy requiring PXR detection at angles Ω closer the electron direction. Near the Bragg condition with a fixed detection location, increasing ϕ produces PXR with greater energy, and this can be achieved through the rotation of the crystal in a rotation stage or goniometer. The last measure that changes the PXR energy also demonstrates the continuous energy tunability of PXR. These measures to change the PXR energy are valid in any geometry, even in back angles ($\Omega > 90^\circ$). However, as detector angles (Ω) increase, the sensitivity of Equation 25 to changes in ϕ reduces the tunable energy range.

Table 9. Measures to increase the PXR energy.

<i>Changed Parameter</i>	<i>Required Action</i>
d -spacing	Reduce d through smaller crystal unit cell or higher (hkl)
ϕ and Ω , at Bragg Condition	Reduce ϕ and Ω , detector closer to electron direction
ϕ , Fixed Detector	Increase ϕ through crystal rotation

2.3.3.4 Energy Uncertainty from Experimental Parameters

The PXR energy width (δE_{PXR}) can be broadened by several physical aspects of the experimental conditions: the electron beam divergence at crystal entrance (θ_{div}); the electron beam multiple scattering in the crystal (θ_{ms}); the electron beam spot diameter (D_e); the crystal thickness (t); the distance from the crystal to the detector (R), the detector collimation width (D_Ω), and the crystal mosaicity (α) [33]. A simple error analysis of Equation 25 shows the following relationship between the three variables used to calculate the PXR energy.

$$\frac{\delta E_{PXR}}{E_{PXR}} = \sqrt{(\cot \phi \cdot \delta \phi)^2 + \left(\frac{\sin \Omega}{1 - \cos \Omega} \delta \Omega \right)^2 + \left(\frac{\delta \tau}{\tau} \right)^2} \quad (26)$$

The uncertainty $\delta \phi$ is related to θ_{Div} and θ_{ms} . The uncertainty in $\delta \Omega$ is related to D_e , t , R , and D_Ω . With exception to pyrolytic graphite, we assume that $\delta \tau$ is negligibly small for perfect crystals. The impact of mosaic spread is discussed later. The electron beam

divergence and multiple scattering have been shown to have second order effects on PXR energy broadening (proportional to θ_{ms}^2 , θ_{div}^2) [34, 33] and these effects are negligible compared to geometric effects. $\delta\phi$ and $\delta\tau$ are approximately zero. The trigonometric terms relating to $\delta\Omega$ can be simplified at the Bragg angle ($2\phi=\Omega$) reducing Equation 26 for spectra taken near the Bragg angle ($\phi=\theta_B$) to the following expression.

$$\frac{\delta E_{PXR}}{E_{PXR}} = \cot \theta_B \cdot \delta\theta_{geo} \quad (27)$$

$\delta\phi$ is replaced by $\delta\theta_{geo}$ defined as the PXR experimental total angular resolution due to geometric effects. $\delta\theta_{geo}$ is approximated as a function of the electron spot size (D_e), the detector collimation (D_Ω), the crystal thickness (t), and the distance to the detector (R). The crystal rotation angle (β) with respects to the electron beam is the dot product ($\hat{n} \cdot \hat{V}$) relating the crystal surface unit normal ($\hat{n}$) and the unit electron velocity ($\hat{V}$) [33].

$$\delta\theta_{geo} \approx \frac{D_\Omega + D_e \cos(\Omega - \beta) + t \sin(\Omega)}{R} \quad (28)$$

Then substituting $\delta\theta_{geo}$ into Equation 27, the energy spread due to geometric effects is given by:

$$\left. \frac{\delta E_{PXR}}{E_{PXR}} \right|_{geo} \approx \frac{D_\Omega + D_e \cos(\Omega - \beta) + t \sin(\Omega)}{R \tan(\Omega / 2)} \quad (29)$$

In determining the energy linewidth effects of beam divergence, multiple scattering, and mosaic spread, the formalism presented by A. P. Potylitsin is considered [34]. To first order, Potylitsin concludes that the electron beam divergence does not effect the PXR energy linewidth and demonstrates this through geometric arguments, which show that the symmetry of the divergence and multiple scattering effects cancel when considered at the extremes defined by $\delta\theta_{geo}$. A.V. Shchagin's PXR technical report on PXR space telescope applications [33] provides a numerical method to calculate the PXR energy linewidth. Shchagin also found beam divergence and multiple scattering to be small compared to the geometric broadening calculated from $\delta\theta_{geo}$.

Potylitsyn [34] derived a generalized expression for energy linewidth that accounts for mosaicity (α) and geometric broadening ($\delta\theta_{geo}$).

$$\left. \frac{\delta E_{PXR}}{E_{PXR}} \right|_{tot} = \cot \theta_B \cdot \sqrt{(\alpha)^2 + (\delta \theta_{geo})^2} \quad (30)$$

For single crystals, α is set to zero. For highly oriented pyrolytic graphite, α is the rocking curve FWHM measured from the Cu K_α emission X-ray.

In order to assess the impact of the geometric and mosaic contributions to the energy linewidth, each of the parameters are considered independently for a common Si(220) PXR experiment with $\theta_B=10^\circ$ and for the typical RPI experimental parameters with the detector 3 m (R) from the crystal. Table 10 summarizes the impact of the various geometric and mosaic properties. For PXR experiments at RPI, the electron spot size is the dominant geometric parameter that broadens the PXR linewidth, and graphite with its mosaicity has the largest impact on the PXR linewidth.

Table 10. The impact of various experimental parameters on the RPI PXR energy linewidth.

<i>Parameter</i>	<i>Dimension</i>	<i>$\Delta E/E$</i>
Spot Size, D_e	1.5 cm	3%
Collimator, D_Ω	3 mm	0.6%
Crystal Thickness, t	500 μm	0.03%
Mosaicity, α	0.4°	4%

Regardless of the geometric broadening terms, the relative energy linewidth is directly related to $\cot(\theta_B)$. The functional relationship of the cotangent is plotted as a function of the Bragg angle, θ_B . This relationship is shown in Figure 18, which demonstrates that for smaller θ_B , the energy linewidth is larger. The geometric energy broadening is smaller at larger Bragg angles.

Figure 18- Bragg angle effect on PXR geometric energy broadening.

2.3.4 Examination of the PXR Photon Yield Characteristics

The photon distribution of PXR at positions near the Bragg angle is typically expressed in the solid angle described by angular displacement from the Bragg condition in the diffraction plane (θ_x) and perpendicular to the diffraction plane (θ_y). While it is common to use units convenient for quantum electrodynamics ($\hbar=c=1$), the MKS expression for the photon distribution of PXR [photons per electron per steradian] is shown in Equation 31 below [11,8].

$$\frac{d^2N}{d\theta_x d\theta_y} = \frac{\alpha}{4\pi} \frac{\omega_B}{c} \left[L_a \left| \frac{\hat{n} \cdot \hat{\Omega}}{\hat{n} \cdot \hat{V}} \right| (1 - e^{-L/(L_a |\hat{n} \cdot \hat{\Omega}|)}) \right] \chi_h^2 e^{-2W} \frac{\theta_x^2 \cos^2 2\theta_B + \theta_y^2}{\sin^2 \theta_B (\theta_x^2 + \theta_y^2 + \theta_{ph}^2)^2} \quad (31)$$

with α the fine structure constant, ω_B the PXR angular frequency, θ_B the Bragg angle, and e^{-2W} is the Debye-Waller term, which relates to the mean lattice vibration ($e^{-2W} \sim 1$ at room temperature). The only term related to the electron energy is θ_{ph} (see Equation 32), the characteristic angle, which defines the spread of the cone of PXR photons. χ_h is the Fourier expansion of the electric susceptibility, which can be viewed as the crystal's diffraction efficiency. The terms in the square brackets are sometimes referred as the "geometric factor" (f_{geo}), and they relate to the photon absorption along the photon escape

path out of the crystal. $\hat{n}$ is the unit normal to the crystal surface, L_a is the absorption length of the PXR in the crystal, and t is the crystal thickness. f_{geo} is discussed in detail later. Both L_a and χ_h depend on the PXR photon energy but in opposing ways. With increased photon energy, L_a increases and χ_h decreases.

2.3.5.1. The Shape of PXR Emission

The distribution of PXR photons is derived from the electric field of the incident relativistic electron. Recall that the electric field is dominated by the component perpendicular to the electron's velocity. This condition results in a unique photon distribution as these virtual photons are diffracted from the crystal planes. The emission cone can be visualized in Figure 19 in which the electron's electric field is shown in its disk-like shape. The PXR emission is the hollow cone centered on vector $\hat{\Omega}$.

Figure 19- Drawing of relativistic electron's disk-like, transverse electric field and hollow cone of PXR emission.

The PXR emission has zero intensity along the vector $\hat{\Omega}$, for the Bragg condition, $\Omega=2\phi$. About the vector $\hat{\Omega}$, the photon distribution has two lobes separated by some characteristic angle, θ_{ph} , determined by the electron energy. As discussed earlier, the X-ray frequency is much greater than the plasma frequency ($\omega \gg \omega_p$) for the crystals used

in these experiments. For electron energies less than 100 MeV, θ_{ph} is approximately γ^{-1} (γ is the Lorentz factor).

$$\theta_{ph} = \sqrt{\frac{1}{\gamma^2} + \left(\frac{\omega_p}{\omega}\right)^2} \quad (32)$$

In Equation 31, the part that defines the photon distribution's shape and polarization is listed below as $N(\theta_x, \theta_y)$.

$$N(\theta_x, \theta_y) = \frac{\theta_x^2 \cos^2 2\theta_B + \theta_y^2}{(\theta_x^2 + \theta_y^2 + \theta_{ph}^2)^2} \quad (33)$$

The shape will be discussed now, and the polarization will be discussed later in the next section. The shape of the distribution can be viewed in a contour plot of the relative intensity. Spacing of contour lines demonstrates the gradient of the intensity change between the lines. Using 60 MeV electrons incident on an arbitrary crystal with $\theta_B=15^\circ$, Figure 20 shows the PXR distribution on the plane normal to the vector $\hat{\Omega}$. This is the perspective of a detector face aligned perpendicular to the PXR emission.

Figure 20- Contour plot of PXR distribution from 60 MeV electrons at perspective normal to the detector face $\hat{\Omega}$.

In Figure 20, the dense lines in the center demonstrate the rapid PXR intensity drop to zero at the Bragg angle. The two lobe intensity maxima can be observed across the θ_y axis, which is perpendicular to the diffraction plane. The more gentle shoulder is observed across the θ_x axis, in the diffraction plane. This can be seen in Figure 21 where Equation 33 is plotted as a function of angular displacement from the Bragg condition in the diffraction plane by setting $\theta_y=0$, and perpendicular to the diffraction by setting $\theta_x=0$. The intensity is normalized to the calculated peak for the perpendicular case. With $\theta_B=15^\circ$, the peak parallel component is about 75% of the perpendicular component, so a point detector would collect the greatest PXR intensity at the position $(\theta_x=0, \theta_y=\theta_{ph})$. For both cases, the peak intensity is observed at an angular displacement known as the characteristic angle $\theta_{ph}=8.7$ mrad away from the Bragg angle. The angular concentration of PXR photons is determined by the electron energy. Higher energy electrons produce a smaller characteristics angle, confining the PXR to a smaller emission cone.

Figure 21- Normalized PXR intensity perpendicular to the diffraction plane ($\theta_x=0$) and in the diffraction plane ($\theta_y=0$) for 60 MeV electrons ($\theta_{ph}=8.7$ mrad).

2.3.5.2. Polarization Of The PXR Emission

The expression defining the shape of the PXR emission also defines the polarization of the PXR emission. θ_x is the parallel component, and θ_y is the perpendicular component of the PXR electric field, respectively [35]. In the numerator of Equation 33, θ_x is weighted by the term, $\cos^2 2\theta_B$. As θ_B approaches 0, the weighting of θ_x approaches unity, and the PXR emission is considered circularly polarized. But as θ_B approaches 45° , the weighting of θ_x approaches zero, and the PXR emission is considered linearly polarized in the perpendicular direction. There is no PXR emission in the diffraction plane at $\theta_B = 45^\circ$. The PXR polarization is demonstrated again with a contour plot of Equation 33 normal to the vector $\hat{\Omega}$. In Figure 22, the vertical direction is perpendicular to the diffraction plane, the horizontal direction is in the diffraction plane. 60 MeV electrons are used.

Figure 22- PXR polarization for $\theta_B = 5^\circ$, 25° and 45° using 60 MeV electrons ($\theta_{ph}=8.7$ mrad).

2.3.5.3. Fourier Transform of Electric Susceptibility

The efficiency of the diffraction of the virtual photons associated with PXR is analogous to the efficiency of diffraction of real photons. Recall from the crystallography discussion in Section 2.1.5, the diffraction efficiency depends on the atomic scattering factor and the crystal plane structure factor. The PXR calculations continue with greater rigor by including corrections for anomalous scattering and thermal lattice vibration. Fortunately, the real and imaginary components of the electric susceptibility, χ , for most crystals considered for this work are well documented and available in a database hosted by Argonne National Laboratory [25]. In an interactive web-supported database called *Xoh*, the methods of Lugovshaya and Stepanov are followed for calculating the real and imaginary components of the polarizabilities, χ_0 and χ_h for ideal absorbing crystals. The database does not provide information about tungsten, W, so the electric susceptibility is calculated locally using the *Xoh* calculation steps. Appendix A shows the steps for calculating the tungsten electric susceptibility and the resources used for the calculation inputs. Once the susceptibilities are determined, χ_0 is used to calculate the crystal's index of refraction and linear attenuation coefficients, while χ_h is used to calculate the crystals diffraction efficiency and the FWHM of the Rocking Curve. Equations for the real and imaginary parts of χ_0 and χ_h are listed below [25]. Parts of Equations 34-37 should be recognized from the discussion of X-ray diffraction in Section 2.1.5. r_0 is the classical radius of the electron, λ is the photon

wavelength, and V is the unit cell volume. N is the net number of atoms in the crystal unit cell. With subscripts j for each of the N atoms, the other terms are σ^D and σ^Q for the crystal atom dipole and quadrupole contributions to the photo-electric absorption; Δf_r for the real part of the atom dispersion correction; $e^{-W(s)}$ for the Debye-Waller term to be discussed in the next section in more detail; and $\vec{r}$ for the position vector of the unit cell atoms.

$$\chi_{0r} = - \left[\frac{r_0 \lambda^2}{\pi V} \right] \sum_{j=1}^N (f_j(0) + \Delta f_{rj}) \quad (34)$$

$$\chi_{0i} = - \left[\frac{\lambda}{2\pi V} \right] \sum_{j=1}^N (\sigma_j^D + \sigma_j^Q) \quad (35)$$

$$\chi_{hr} = - \left[\frac{r_0 \lambda^2}{\pi V} \right] \sum_{j=1}^N e^{-W_j(s)} (f_j(s) + \Delta f_{rj}) e^{i\vec{r} \cdot \vec{r}_j} \quad (36)$$

$$\chi_{0i} = - \left[\frac{\lambda}{2\pi V} \right] \sum_{j=1}^N e^{-W_j(s)} (\sigma_j^D + \sigma_j^Q) e^{i\vec{r} \cdot \vec{r}_j} \quad (37)$$

For single element crystals, the summations in the equations for χ_0 are simply the product of the number of unit cell atoms, N , and the remaining summed quantities. The exponential part of the summations in the equations for χ_h are simply the structure factor, S_{hkl} , defined earlier in Equation 7. χ_0 has no structure dependence. For most crystals considered for this research, the web database was used as the resource for χ_0 and χ_h . In particular, χ_{0i} is used to determine the linear attenuation coefficient, μ_{tot} . χ_{hr} and χ_{hi} are used to determine χ_h^2 . Their specific uses are shown below

$$\mu_{tot} = \frac{2\pi |\chi_{0i}|}{\lambda} \quad (38)$$

$$\chi_h^2 = \chi_{hr}^2 + \chi_{hi}^2 \quad (39)$$

An example output from this database is shown in Appendix B. A local database is generated for this work by collecting χ_{0H} output for 15-20 discrete X-ray energies 5-100 keV, and interpolating the χ_0 , χ_{hr} , and χ_{hi} values between energies. At energies near an

absorption edge, the selected discrete energies used for the χ_{oH} output are selected to provide resolution just above and below the edge. The values for χ_h^2 and μ_{tot} help determine the PXR yield due to production efficiency and photon absorption in the crystal, respectively. Both terms decrease with PXR energy meaning less production, but less loss in the crystal. However, with an increase in PXR energy, χ_h^2 decreases more rapidly than μ_{tot} . Figure 23 shows χ_h^2 and μ_{tot} for Silicon (220) plotted as a function of PXR energy. Quantities are normalized to values at 5 keV for comparison.

Figure 23- χ_h^2 and μ_{tot} for Si(220) normalized to values at 5 keV.

To appreciate the impact of the differences in χ_h^2 and μ_{tot} at different PXR energies, a more detailed study of the photon crystal escape path is necessary.

2.3.5.4. Photon Losses in the Crystal

PXR is produced per unit length as the electron interacts with subsequent crystal unit cell volumes. The geometric factor (f_{geo}) has the dimensions of length, and it represents the photon absorption along the escape path out of the crystal [36].

$$f_{geo} = L_a \left| \frac{\hat{n} \cdot \hat{\Omega}}{\hat{n} \cdot \hat{V}} \right| (1 - e^{-t/(L_a |\hat{n} \cdot \hat{\Omega}|)}) \quad (40)$$

The derivation of this term is shown in Appendix C for an arbitrary crystal surface orientation to the chosen crystallographic plane. For this derivation, the electron is assumed to travel along a straight line through the crystal with negligible scattering. Recall that a term was introduced earlier for the distance the electron travels in the crystal to loss a factor of e^{-1} of its energy through collision and radiation losses. We called that length the energy loss length, X . To test of the validity of this assumption, the electron energy loss length, X , for 60 MeV electrons are compared in Table 11 to the 15 keV photon absorption lengths (L_a) for the example crystals. X is much greater than L_a for each of the example crystals.

Table 11. Total energy loss from electron crystal interactions

<i>Crystal</i>	<i>Energy Loss Length, X [mm]</i>	<i>Absorption Length, L_a [mm]</i>
Graphite	114	9.14
Lithium Fluoride	75	1.57
Silicon	61	0.44
Tungsten	3.4	0.0038

The geometric and energy dependence of f_{geo} are now considered. Three distinctive orientations are shown in Figure 24. In the *Bragg* geometry the diffraction planes are parallel to the crystal surface, and in the *Laue* geometry the diffraction planes are perpendicular to the crystal surface. The *Asymmetric Laue* geometry is a combination of the Bragg and Laue geometries in which the diffraction planes make an angle of 45° to the surface of the crystal.

Figure 24- Different crystal plane orientations to the crystal surface. Bragg, Laue, and Asymmetric Laue geometries for comparable ϕ , $\vec{V}$, and $\hat{\Omega}$.

Although Figure 24 is not drawn to scale, the relative angles between the vectors used to calculate f_{geo} are demonstrated. The photon escape path length and electron interaction path length can be qualitatively assessed for the three geometries. These lengths are a function of the crystal dimensions, but for the moment assume that the crystal thickness t is much smaller than its diameter, D ($t \ll D$). In Table 12, the vector dot products $\hat{n} \cdot \hat{\Omega}$ and $\hat{n} \cdot \hat{V}$ are evaluated as a function of the incident angle ϕ . Qualitative comparisons of the photon and electron path lengths are made for $\phi < 45^\circ$. The photon path length is inversely proportional to $\hat{n} \cdot \hat{\Omega}$; the photon path length is directly proportional to $\hat{n} \cdot \hat{V}$.

Table 12. Comparison of f_{geo} vector products and photon/electron crystal path lengths for the Bragg, Laue, and Asymmetric Laue geometries

<i>Geometry</i>	$\hat{n} \cdot \hat{\Omega}$	$\hat{n} \cdot \hat{V}$	<i>Photon Path</i>	<i>Electron Path</i>
Bragg	$\sin(\phi)$	$\sin(\phi)$	greatest, $\phi < 22.5^\circ$	greatest
Laue	$\cos(\phi)$	$\cos(\phi)$	least	least
Asymmetric Laue	$\sin(\pi/4 - \phi)$	$\cos(\pi/4 - \phi)$	greatest, $\phi > 22.5^\circ$	intermediate

For any fixed geometry, the functional nature of f_{geo} is to saturate at the value of the absorption length, $L_a = \mu_{tot}^{-1}$. Consider the three geometry cases, the example Si (220) material, and a PXR energy of 15 keV with $L_a = 440 \mu\text{m}$, and $\phi = \theta_B = 12.4^\circ$ for Si(220). Assume all three geometries are commercially available. The most efficient geometry for producing PXR can be assessed by evaluating f_{geo} as a function of crystal thickness. In Figure 25, the normalized f_{geo} (f_{geo}/L_a) is plotted as a function of crystal thickness in units of absorption lengths, L_a .

Figure 25- Normalized f_{geo} evaluated as a function of crystal thickness for the Bragg, Laue, and Asymmetric Laue geometries in the case of Si (220) and 15 keV PXR.

Although Figure 25 is specific to a unique ϕ , material, and PXR energy, it is presented in a generic fashion that makes it applicable for most any ϕ up to 45° and any material. The Asymmetric Laue geometry saturates at a value lower than L_a , which reduces the PXR yield to about 60% of what can be achieved at this 12.4° Bragg angle. For this reason, the *Asymmetric Laue* geometry is generally not used for PXR production. For both the *Bragg* and *Laue* geometries, the f_{geo} achieves the maximum value of L_a but at different crystal thickness. f_{geo} saturates at a crystal thickness of about one absorption length for the *Bragg* geometry and four absorption lengths for the *Laue* geometry. In other words, about four times more target crystal thickness is needed in the *Laue* geometry to produce the same yield as in the *Bragg* geometry. This may make the choice of *Bragg* geometry obvious. It is important to note that these conclusions ignore the effect of the crystal thickness on the electron beam, but the analysis is appropriate for the conditions $X_o \gg L_a$. There are some trade-offs in other design parameters such as the need to minimize bremsstrahlung from the target crystal, which may make the *Laue* geometry more attractive. This will be discussed later in Chapter 4.

Now consider the effects of photon energy on f_{geo} . Even if the geometry is optimized in terms of orientation of planes and crystal thickness, the maximum value of f_{geo} is still constrained to L_a . Absorption length depends on the PXR photon energy. For a given crystal, the absorption length ($L_a = \mu_{tot}^{-1}$) increases with photon energy. Figure 23 highlighted the rate of change in μ_{tot} and χ_h^2 with photon energy. Figure 26 shows L_a and χ_h^2 for Si (220) for varying energy.

Figure 26- L_a and χ_h^2 for Si (220) plotted as a function of PXR energy.

The nature of their energy relationship demonstrates the strong dependence of the PXR yield on the product of L_a and χ_h^2 . Calculation of the total integrated PXR photon yield is done using all terms of Equation 31 except the shape term. Figure 27 shows the total integrated yield as a function of energy. Plots for Si (220) with thickness 0.5 mm, 1.0 mm, and 2.0 mm are shown for discussion.

Figure 27- Si(220) integrated yield from crystals with varying thickness in Laue geometry.

In the low energy region, the three graphs coincide. Under this condition, f_{geo} is approximately L_a for those energies; at these energies, the thickness of each crystal is at least four L_a . Note that for Bragg geometry, a crystal thickness of only one L_a is needed to saturate f_{geo} and the yield continues on a climbing slope for a much broader energy region. Returning to the Laue geometry at higher energies, the yields diverge from each other, continue on a rising slope to a maximum value, and then begin to fall off. The rising edge represents the dominant influence of increasing values for L_a . The maximum values occur at energies when the crystal thickness approximately equals L_a . The falling edge of the yield represents the dominant influence of χ_h^2 , which decreased more rapidly than L_a . Thicker crystals produce more PXR beyond the energy region where the yields begin to diverge, and for a given crystal thickness, there is an energy that produces the maximum PXR yield.

2.3.5.5. Effects of Crystal Heating

The Debye-Waller term e^{-2W} in Equation 31 accounts for the PXR phase loss due to thermal lattice vibrations. This effect is dependent on the material specific Debye temperature, T_D , the material physical temperature, T , and the d-spacing of the diffraction

plane of interest, d_{hkl} . The first quantity of interest is the mean square amplitude of the thermal vibration of the crystal, $u(T)^2$. This can be calculated using the expression below [37] where $\hbar$ is plank's constant divided by 2π , A is the material mass number, and k_B is the Boltzman constant. y is an integration variable.

$$u^2(T) = \frac{3\hbar}{4Ak_B T_D} \left[1 + 4 \left(\frac{T}{T_D} \right)^2 \left(\int_0^{T_D/T} \frac{y dy}{e^y - 1} \right) \right] \quad (41)$$

The Debye-Waller term is calculated from $u(T)^2$ and the reciprocal lattice vector $\tau = 2\pi/d_{hkl}$ using the following relationship [37].

$$e^{-2W} = \exp[-u^2(T)(\tau)^2] \quad (42)$$

An equivalent expression for the mean square amplitude of the thermal vibration is listed below by using the Debye function, $\phi(x)$, which contains all of the temperature dependence of the Debye-Waller term [6] with the $x = T_D/T$.

$$u^2(x) = \frac{9.76 \cdot 10^6 \cdot \lambda^2}{AT_D} \left\{ \frac{\phi(x)}{x} + \frac{1}{4} \right\} \quad (43)$$

$$\phi(x) = \frac{1}{x} \int_0^x \frac{y dy}{e^y - 1} \quad (44)$$

For decreasing x , the temperature is increasing. Debye temperatures, T_D , are typically a few hundred K, so crystal cooling may allow values of x up to 10 and heating can drive x down to perhaps as low as 1/3 where the crystal material is likely to melt or ignite. Figure 28 shows the shape of the Debye function for values of x up to 10. For $x=1$, $T=T_D$ and the Debye function $\phi(1)=0.778$. Conditions that minimize $\phi(x)$ are desired for PXR production.

Figure 28- Debye function $\phi(x)$ versus x , where $x=T_D/T$.

In order to gain an appreciation of the magnitude of the Debye-Waller Factor, Equation 42 is used to calculate the intensity reduction factor for Si (220) and LiF (220) for varying temperatures. In Figure 29, it is shown that thermal lattice vibrations exist down to low temperatures approaching absolute zero, $T=0^\circ$ K. Additionally, there are apparent differences in the Debye-Waller Factor between the two crystals. The ratio between the LiF and Si Debye temperatures is 1.4 while the ratio between τ^2 for LiF and Si is 1.8. The Debye-Waller Factor is more affected by changes in τ^2 so the difference between the two crystals is primarily associated with the smaller d-spacing for LiF (220). Finally, the X_{oh} database makes calculations that include the Debye-Waller Factor at room temperature, $T=300^\circ$ K. Consequently, any corrections made for the increased crystal temperature should be scaled by the ratio of Debye-Waller Factor at $T=300^\circ$ K to that at the elevated temperature.

Figure 29- Calculated Debye-Waller Factor for Si (220) and LiF (220).

2.3.5 Calculated PXR Yield for Various Crystals

In this section, the method for calculating the PXR yield at a detector location is presented. The method is then used to calculate the yield for a variety of target crystals, which is then compared for the production of PXR at different energies.

2.3.5.1. Calculation Method for PXR Yield in the Detector Solid Angle.

The PXR yield N (photon/e/solid angle) is calculated by integrating the differential PXR yield, Equation 31, about the detector solid angle defined by $d\theta_x$ and $d\theta_y$.

$$N = \iint_{\theta_y, \theta_x} \frac{\alpha}{4\pi} \frac{\omega}{c} \left[L_a \left| \frac{\hat{n} \cdot \hat{\Omega}}{\hat{n} \cdot \hat{V}} \right| \left(1 - e^{-L/(L_a |\hat{n} \cdot \hat{\Omega}|)} \right) \right] \chi^2 e^{-2W} \frac{\theta_x^2 \cos^2 2\theta_B + \theta_y^2}{\sin^2 \theta_B (\theta_x^2 + \theta_y^2 + \theta_{ph}^2)^2} d\theta_x d\theta_y \quad (45)$$

The detector solid angle, Ω , is determined from the distance R from the crystal to the detector face, and Δx and Δy the detector linear dimensions in the diffraction and perpendicular to the diffraction plane, respectively. An expression for the detector solid angle is shown below [28].

$$\Omega \approx \frac{Area}{R^2} = \frac{\Delta x \cdot \Delta y}{R^2} \quad (46)$$

The dimensions of Δx and Δy are often constrained by the aperture of the detector collimator. Future discussions refer to Δx and Δy as the collimation dimensions. For the conditions where $\Delta x, \Delta y \ll R$, the small angle approximation applies, and $d\theta_x = \Delta x/R$ and $d\theta_y = \Delta y/R$. Because the PXR intensity is greatest at $\theta_x = 0$ and $\theta_y = \theta_{ph}$, the detector should be centered at this position. Then the integration limits on $d\theta_x$ and $d\theta_y$ are determined below.

$$\left(\frac{-\Delta x}{2R} \right) \leq d\theta_x \leq \left(\frac{\Delta x}{2R} \right) \quad (47)$$

$$\left(\theta_{ph} - \frac{\Delta y}{2R} \right) \leq d\theta_y \leq \left(\theta_{ph} + \frac{\Delta y}{2R} \right) \quad (48)$$

The PXR yield for a particular experimental geometry is calculated with the integration of Equation 45 using these integration limits. Appendix D shows the use of the χoh database information with an example calculation used to determine the Si(220) PXR yield for 15 keV photons.

2.3.5.2. Calculated PXR Yield for Various Crystals and Planes.

A list of potential PXR crystal was developed after a search of the literature on PXR and X-ray optics. The materials considered for PXR production are listed below in order of their atomic number, Z . Other material specific parameters to include the lattice type, unit cell dimensions, ρ the mass density, ρ_e the charge density, ω_p the plasma frequency, and the T_D the Debye temperature are all listed for comparison [38, 16, 39, 40].

Table 13. General Characteristics of PXR crystal materials.

<i>Material</i>	<i>Z</i>	<i>Lattice</i>	<i>Unit Cell</i> [Å]	ρ [g/cm ³]	ρ_e [e/cm ³]	ω_p [rad/s]	T_D [°K]
Be	4	Hex	d ₀ =2.552 c=3.583	1.84	4.94x10 ²³	3.96x10 ¹⁶	1000
Graphite	6	Hex	d ₀ =2.461 c=6.708	2.26	6.82x10 ²³	4.66x10 ¹⁶	1860
Diamond	6	FCC	d ₀ =3.567	3.54	1.07x10 ²⁴	5.82x10 ¹⁶	1860
LiF	8.3	FCC	d ₀ =4.026	2.64	7.34x10 ²³	4.84x10 ¹⁶	730
Si	14	FCC	d ₀ =5.431	2.33	6.99x10 ²³	4.74x10 ¹⁶	625
Cu	29	FCC	d ₀ =3.615	8.97	2.46x10 ²⁴	7.68x10 ¹⁶	315
Ge	32	FCC	d ₀ =5.658	5.32	1.41x10 ²⁴	6.70x10 ¹⁶	360
W	74	BCC	d ₀ =3.165	19.30	4.68x10 ²⁴	12.69x10 ¹⁶	310

Information listed in Table 13 allows for some specific crystal plane parameters to be calculated. This is the start of the comparison of crystal material and crystal planes selected to optimize PXR production at a particular PXR energy. In Table 14, the crystal plane d-spacing (d_{hkl}) and the energy specific parameters absorption length (L_a), electric susceptibility (χ_H), and the Bragg angle (θ_B) are listed for 15 keV PXR.

Table 14. Specific Crystal Plane Characteristics for 15 keV PXR.

<i>Crystal Plane</i>	d_{hkl} [Å]	L_a [μm]	χ_H [10 ⁻⁶]	θ_B [Deg]
Be (002)	1.79	20759.0	1.300	13.34
Graphite (002)	3.35	9144.3	3.101	7.09
Diamond (111)	2.05	5849.5	2.368	11.60
LiF (200)	2.01	1568.8	2.768	11.84
LiF (220)	1.42	1568.8	1.978	16.87
Si (111)	3.14	443.7	2.271	7.57
Si (220)	1.92	443.7	2.601	12.43
Cu (111)	2.08	15.0	11.368	11.44
Ge (111)	3.27	20.5	5.183	7.27
W (110)	2.24	3.8	23.240	13.07
W (222)	0.91	3.8	18.940	26.88

Recall that the PXR yield depends on L_a and χ_H^2 . The atomic number of the crystal is important in determining these parameters. In general, PXR production efficiency is proportional to Z^2 , but the PXR absorption length decreases proportional to Z^{-4} , where Z is the crystal atomic number Z [5]. For higher Z materials, the absorption losses increase more rapidly than the PXR production [41]. This makes low Z target crystals preferable to high Z crystals for lower energy (<20 keV) PXR production. This can be seen in Table 14 by comparing the values for Be (002) and W(110). Be is nearly transparent to the 15 keV photons, while these photons are heavily absorbed by W. Nonetheless, χ_H for W(110) is nearly 18 times greater than that for Be (002) producing greater than two orders of magnitude more 15 keV photons. The other distinction between crystals lies with the distance between planes. The d-spacing for Graphite (002) is nearly four times larger than the d-spacing for W (222). Consequently, the W (222) Bragg angle is nearly four times greater than that for Graphite (002). The larger d-spacing may be problematic since smaller Bragg angles demand PXR detection at angles closer to the electron beam path. For the experiments at RPI, the detection angle has arbitrarily set to angles greater than 9° so that the minimum acceptable Bragg angle is 4.5°.

If there were no other constraints, then the PXR experiments would be performed with the crystal that produced the maximum number of photons at a given energy. Consider the idealized case for four of the crystals in Table 14. Then the crystals would have a thickness of one L_a . Their PXR yield would be compared in the Bragg geometry, which was shown in Figure 25 to reach a saturation point near a crystal thickness of one L_a . The PXR yield [photons/e/mm²] is calculated for three PXR energies, 15, 30, and 60 keV with the crystal thickness of one L_a . The different crystals will have different thickness based on the corresponding L_a for that PXR energy. The energy is varied by changing the electron incident angle (ϕ) measured with respect to the crystal planes, and the PXR emission angle (Ω) is adjusted to preserve the Bragg Condition, $\Omega=2\phi$ around which produces the maximum PXR intensity. The calculation assumptions are 60 MeV electrons and the detector collimation is 1 mm x 1mm at a distance $R=1m$. Table 15 shows the crystal planes: Be (002), Si (220), LiF (220), and W (110) and their corresponding absorption length L_a , Bragg angle θ_B , and photon yield for the three selected PXR energies.

Table 15. Idealized Be, Si, LiF and HOPG Crystal PXR Yield [photon/e/mm²] for thickness L_a at energies 15, 30, and 60 keV.

<i>Crystal</i>	<i>15 keV</i>			<i>30 keV</i>			<i>60 keV</i>		
	L_a [mm]	θ_B [deg]	Yield [ph/e/mm ²]	L_a [mm]	θ_B [deg]	Yield [ph/e/mm ²]	L_a [mm]	θ_B [deg]	Yield [ph/e/mm ²]
Be (002)	21.000	13.3	9.50E-08	158.000	6.6	3.78E-07	1070.000	3.3	1.28E-06
Si (220)	0.444	12.4	9.22E-09	3.614	6.2	3.90E-08	29.650	3.1	1.61E-07
LiF (200)	1.568	11.8	4.06E-08	13.600	5.9	1.85E-07	117.370	4.2	8.06E-07
W (110)	0.004	10.6	6.46E-09	0.024	5.3	2.70E-08	0.164	2.6	9.37E-08

Table 15 brings out some interesting points. Even with the small W (110) d-spacing, small Bragg angles severely constrain the production of 30 and 60 keV PXR because of the complications of detection near the electron beam path. Higher order reflections have smaller d-spacing and can produce higher energies and more easily achieved Bragg angles. However, this comes with a reduction in χ_H^2 and typically two orders of magnitude reduction in photon yield. For a given crystal plane, higher photon yields are

achieved for higher PXR energies. This is primarily attributable to the increase in L_a and to a lesser extent the increase in ω . Despite the complications with small Bragg angles, the beryllium crystal produces the greatest 60 keV photon yield, but this is with an unreasonable crystal thickness greater than 1 m; this is a thickness of about three Be radiation lengths ($3X_o$), which would have a substantial impact on the electron beam multiple scattering. Additionally, Beryllium single crystals are not available in any of the thickness L_a shown in the Table 15. Be is abandoned from future consideration for PXR production because of its availability and the effect that its thick slab-like dimensions would have on the electron beam. While relatively thin, tungsten crystals with thickness L_a are not commercially available in single crystal form; a 1 mm thickness is available [40]. While idealized analysis of crystal thickness and experimental geometries should be considered, the plan for PXR experiments must be grounded with the realities of available crystals and reasonable experimental set-up.

After consulting a number of commercial crystal and wafer vendors, it was concluded that 1 mm thickness was readily available for most single crystals and 0.5 mm for polished wafers. A comparison of the on-hand crystals was done with thickness 1 mm, Bragg geometry, and 60 MeV electrons. The exception was with Ge and Si which both had thickness 0.5 mm. The energy is varied by changing the electron incident angle (ϕ) measured with respect to the crystal planes, and the PXR emission angle (Ω) is adjusted to preserve the Bragg Condition, $\Omega=2\phi$. Again, the calculation assumptions are 60 MeV electrons, and the detector collimation is 1 mm x 1mm at a distance $R=1\text{m}$. Ω is kept greater than 9° .

Figure 30- PXR photon yield for on-hand PXR crystals HOPG, LiF, Si, Cu and W.

Figure 30 can be used as an experimental planning guide for selecting the crystal and plane best suited for producing a given PXR energy. Clearly, for photon energies less than 20 keV, graphite produces the greatest number of photons beating its next best competitor, LiF (200) by nearly an order of magnitude. However, the graphite large d-spacing limits its practical use to lower energies. Beyond 20 keV, the LiF and Si crystal planes produce more photons than the metallic Cu and W crystals. But like graphite, the LiF and Si lose practical use at about 40 keV because the PXR will be emitted in the electron beam direction. At these higher energies, the Cu and W become more favorable.

2.3.6 Photon Distribution Broadening

Early in the development of the theory, Feranchuck and Ivanshin developed the expression for the differential photon yield N , per unit solid angle, per frequency ω [42].

$$\frac{d^2N}{d\theta_x d\theta_y d\omega} = \frac{1}{2\pi^2} \frac{e^2}{\hbar c} \frac{1}{\omega_B} \chi^2 \frac{\theta_x^2 \cos^2 2\theta_B + \theta_y^2}{(\theta_x^2 + \theta_y^2 + \theta_{ph}^2)^2} \frac{1}{16 \sin^4 \theta_B \left(\frac{\theta_x}{\tan \theta_B} - \frac{\Delta\omega}{\omega_B} \right) + \rho_s^2} \quad (49)$$

ρ_s is a photon interaction probability in the crystal, $\rho_s = \lambda / (L_a 2\pi)$. This early theoretical consideration was the first to add some mechanism that broadens the distinctive two-lobe PXR photon distribution. The differential yield in Equation 31 comes partially from the integration of Equation 49 over all ω in the PXR solid angle.

A visualization of the possible distribution broadening is shown in Figure 31. The dimensions are not drawn to scale. In this case, the crystal thickness, t , is depicted such that the PXR distribution from the crystal front surface is shown superimposed with the PXR distribution from the crystal back surface. The effect at the detector is the filling of the minima at the Bragg angle.

Figure 31- Visualization of distribution broadening due to physical conditions of experiment. Dimensions are exaggerated.

There are two approaches for applying the experimental conditions to the calculation of the PXR photon distribution. The first approach by Feranchuck-Ivashin

[42] adds a broadening term to θ_{ph} in Equation 31, and the second by Potylitsyn [34] convolutes Equation 31 with a gaussian distribution that accounts for beam divergence and crystal mosaicity. Recall that without broadening, Equation 33 defines the shape of the distribution. This will be used to compare the two approaches for broadening and the shape perpendicular to the diffraction plane ($\theta_x=0$) will be presented.

In the Feranchuck-Ivashin method, the electron beam divergence (σ_e) results from the divergence at entrance (θ_{div}) to the crystal and multiple scattering (θ_{ms}) in the crystal. The two effects add in quadrature so that σ_e is determined below.

$$\sigma_e^2 = \theta_{div}^2 + \theta_{ms}^2 \quad (50)$$

Then the Feranchuck-Ivashin method would determine N , the photon distribution, resulting from beam divergence with the following expression.

$$N(\theta_x, \theta_y, \sigma_e) = \frac{\theta_x^2 \cos^2 2\theta_B + \theta_y^2}{(\theta_x^2 + \theta_y^2 + \theta_{ph}^2 + \sigma_e^2)^2} \quad (51)$$

Figure 32- Feranchuck-Ivashin Method for PXR broadening. Calculation done with $\theta_x=0$ and θ_y normalized to values of θ_{ph} .

In Figure 32, there is a flattening of the photon distribution and broadening that shifts the peak to the angle $\theta_y = \theta_{ph} + \alpha$. The flattening is consistent with experimental results reported in the literature [43]. However, this method does not demonstrate the filling of

minima at the Bragg angle, and it over estimates the effects of the broadening mechanism in thick crystals [44].

The Potylitsyn method allows the calculation of the broadening effects from beam divergence and crystal mosaicity all in a single expression that relates the PXR unbroadened distribution (Equation 33) and gaussian convolutions from the two effects. The gaussian distribution for the beam divergence has standard deviation σ_x and σ_y in the diffraction plane and perpendicular to the diffraction plane, respectively. The beam divergence can be characterized using the following expression with C_e defined as a normalization constant and $\Delta x, \Delta y$ angular positions about the Bragg angle.

$$G_m(\Delta x, \Delta y) = C_e \exp\left\{\frac{\Delta x^2}{2\sigma_x^2}\right\} \exp\left\{\frac{\Delta y^2}{2\sigma_y^2}\right\} \quad (52)$$

Note that when the electron emittance is known, its components are used for the different components of σ . At RPI, the electron beam emittance is not known. But with the 10-mil Be window, we assume that the electron divergence at the crystal entrance is small compared to multiple scattering in the crystal. We assume that $\sigma_x = \sigma_y = \sigma_{ms}$, the standard deviation of the electron beam multiple scattering angle. Similarly, the crystal mosaicity with standard deviation σ_m can be characterized using the following expression with C_m defined as another normalization constant and α_x, α_y angular positions about the Bragg angle.

$$G_m(\alpha_x, \alpha_y) = C_m \exp\left\{\frac{\alpha_x^2}{2\sigma_m^2}\right\} \exp\left\{\frac{\alpha_y^2}{2\sigma_m^2}\right\} \quad (53)$$

New variables are defined such that $\xi_x = \Delta x - 2\alpha_x$ and $\xi_y = -\Delta y + 2\alpha_y \sin(\theta_B)$. This allows the two gaussian distributions to be combined into a single effective gaussian $G(\xi_x, \xi_y)_{e,m}$ that evaluates the two effects. In the equation below, $C_{e,m}$ is a normalization constant; ξ_x and ξ_y correspond to angular displacement from the Bragg angle in and perpendicular to the diffraction plane, respectively.

$$G(\xi_x, \xi_y)_{e,m} = C_{e,m} \exp \left\{ \frac{\xi_x^2}{2\sigma_x^2 \left(1 + 4\sigma_m^2 / \sigma_x^2 \right)} \right\} \exp \left\{ \frac{\xi_y^2}{2\sigma_y^2 \left(1 + 4\sin^2(\theta_B) \sigma_m^2 / \sigma_y^2 \right)} \right\} \quad (54)$$

The additional terms in the denominator are derived from geometric consideration and the shift in variables. The exponentials in $G(\xi_x, \xi_y)_{e,m}$ provide some insight about the relative magnitudes of the two effects. The effective standard deviation in the x direction is $\sqrt{\sigma_x^2 + 4\sigma_m^2}$ and $\sqrt{\sigma_y^2 + 4\sigma_m^2 \sin^2(\theta_B)}$ in the y direction. In the x direction, the mosaicity is weighted four times more than the beam divergence; in the y direction the relative weighting depends on the Bragg angle.

The convolution of the PXR shape term with $G(\xi_x, \xi_y)_{e,m}$ integrated over appropriate limits then determines the broadening caused by beam divergence and mosaicity. The expression below is used.

$$A_{e,m}(\theta_x, \theta_y) = \iint G(\xi_x, \xi_y)_{e,m} N(\theta_x + \xi_x, \theta_y + \xi_y) d\xi_x d\xi_y \quad (55)$$

In subsequent calculations, four standard deviations ($4\sigma_e$ and $4\sigma_m$) are used for the integration limits on the gaussian distributions for the electron beam divergence and the crystal mosaicity. With these values and setting $C_{e,m}$ temporarily to one, Equation 55 is integrated about two standard deviations of ξ_x and ξ_y using the following limits:

$$\begin{aligned} -2\sqrt{\sigma_x^2 + 4\sigma_m^2} \leq \xi_x \leq 2\sqrt{\sigma_x^2 + 4\sigma_m^2} \\ \text{and} \\ -2\sqrt{\sigma_y^2 + 4\sigma_m^2 \sin^2(\theta_B)} \leq \xi_y \leq 2\sqrt{\sigma_y^2 + 4\sigma_m^2 \sin^2(\theta_B)} \end{aligned} \quad (56)$$

The normalization constant $C_{e,m}$ is determined by comparing the integrated area under the curve formed by Equation 55 (distribution with broadening) and the integrated area under the curve formed by Equation 33 (distribution without broadening). The specific steps for this calculation are shown in Appendix E. To demonstrate the impact of

electron beam divergence and crystal mosaicity, the two effects are considered separately using Equation 55. The calculations are plotted below for the following parameters: $\theta_{ph}=8.5$ mrad (60 MeV electrons), $\theta_y=0$, and $\theta_B=15^\circ$. For examining the electron beam divergence, the crystal mosaicity was set to zero ($\sigma_m=0$), and for examining the crystal mosaicity, the electron beam divergence was set to zero ($\sigma_e=0$). The plots are normalized to the area under the un-broadened curve.

Figure 33- Electron divergence effects on PXR photon distribution. Calculations done as a function of θ_x and with $\theta_{ph}=8.5$ mrad, $\theta_y=0$, $\theta_B=15^\circ$, no crystal mosaicity ($\sigma_m=0$), and varying values of $\sigma_e=(0,0.25, 0.5, 1.0)*\theta_{ph}$.

Figure 34- Crystal mosaic effects on PXR photon distribution. Calculations done as a function of θ_x and with $\theta_{ph}=8.5$ mrad, $\theta_y=0$, $\theta_B=15^\circ$, no electron beam divergence ($\sigma_e=0$), and varying values of $\sigma_m=(0,0.25, 0.5, 1.0)*\theta_{ph}$.

In Figures 33-34, the filling of the PXR distribution near the Bragg angle occurs as expected. Additionally, these normalized curves demonstrate that the width (FWHM) of the curves is not changed with larger values of beam divergence or crystal mosaicity. These effects will be considered when comparing experimental data with predicted values.

CHAPTER 3

EXPERIMENTAL COMPONENTS

3.1 GAERTTNER LINEAR ACCELERATOR

This chapter is divided into five sections. The first two sections discuss the RPI LINAC and systems for monitoring the electron beam energy, current, position, and shape. The next section is devoted to the PXR crystals. This is followed by the detection systems. The chapter ends with figures that describe the overall experimental set-up and scheme for data acquisition.

3.1.1. General Characteristics

The Gaertner linear accelerator (LINAC) at Rensselaer Polytechnic Institute (RPI) accelerates electron to energies up to 60 MeV. The RPI LINAC is primarily used for neutron cross-section measurements. Other uses are for medical isotope production, gamma activation analysis, and now PXR production. The accelerator operates in the L-band (1.300 GHz), which results in RF radio frequency wavelength of 23.0 cm. The physical dimensions of the LINAC depend on the operating frequency. The RF waveguides operate in a transverse electric (TE) mode and have a quarter wave transverse amplitude dimension (total width is $\lambda/2=11.5$ cm). The electron acceleration sections operate in the transverse magnetic (TM) mode, and most have $\pi/2$ cavity design, which modulates the longitudinal electric field amplitude. These acceleration sections are four wavelengths long ($4\lambda=92$ cm) with the a $\pi/2$ cavity every wavelength [51]. By comparison, other more common LINACs operate in the S-Band (2.600 GHz), which affords a more compact design with wavelength of 11.5 cm [45].

The RPI LINAC originally had nine acceleration sections with a single output window from which the electrons exited. In the mid 1980's, the forth section was removed so that an additional output window could be installed after the third section. The fourth section was displaced to the end of the LINAC so that there remained a total of nine sections. Figure 35 shows the general layout of the RPI LINAC. This is not drawn to scale. The LINAC now can produce electrons from a low energy port and a high-energy port. The electron gun produces the electrons to be accelerated by the

LINAC. Applied Radiation Corporation (ARCO) manufactured the existing gun, and its cathode voltage is 80-100 kV. After some initial electron bunching system, the electrons are accelerated in nine LINAC sections with pulses of RF energy injected from nine separate klystrons.

The low energy port immediately follows the first three sections. A bending magnet (M1) with peak field strength of 4.260 Gauss at 29 amperes deflects the electrons approximately 30° laterally to the right to the low energy output window. The actual deflection angle is dependent on the electron beam energy distribution and the magnetic field profile. The LINAC technicians vary the magnet current in order to optimize the experimental conditions. When bending magnet M1 is off, the electrons continue through the remaining six LINAC sections. An additional ARCO analyzer magnet (M2) used to measure the electron energy deflects the electrons approximately 22.5° laterally to the left. A Faraday cup is positioned behind a 1/4" slit, and the current in M2 is varied until the maximum signal is observed at the Faraday cup. The electron energy is determined using energy calibrations provided by ARCO. When bending magnet M2 is off, the electrons continue in vacuum without further acceleration except for interaction with two additional quadrupole magnets Q1, Q2. Rather than focusing the electron beam, these magnets are wired so that the two south poles are adjacent and the two north poles are adjacent so that the effect is to steer left/right and up/down.

Figure 35- Schematic of the RPI LINAC. The nine accelerator sections are shown with two possible electron output after three and nine sections. Not drawn to scale.

The RPI LINAC technicians operate the accelerator during PXR experiments. The LINAC is tuned at the start of each PXR experiment. Tuning involves monitoring the electron beam current measured from the collection of charge on an insulated lead brick with sufficient thickness to stop 60 MeV electrons (2" thick). PXR instruments are removed from the LINAC target room during the tuning process. Typically, 1 μA is

needed to optimize the controls available to the LINAC technicians. The general controls available are electron steering with use of the quadrupole magnets (Q1, Q2), adjustments of the electron beam current with changes in the gun injector voltage, and electron pulse rate and pulse width with changes in the klystrons. There are two options (short and long) for pulsing the capacitor banks associated with the klystrons. Table 16 shows the general capabilities of the RPI LINAC from the two configurations for electron output.

Table 16. General RPI LINAC capabilities from the low and high-energy ports.

<i>Capability</i>	<i>Three Sections</i>	<i>Nine Section</i>
	(Low Energy Port)	(High Energy Port)
Electron Energy	5 to 25 MeV	25 to over 60 MeV
Pulse Width	15 to 5000 ns	15 to 5000 ns
Peak Current	3A (short pulse: 15 to 50 ns) 400 mA (long pulse: 50 to 5000 ns)	3A (short pulse: 15 to 50 ns) 400 mA (long pulse: 50 to 5000 ns)
Max Average Power	10 kW@ 17 MeV, 5000 ns	10 kW@ 60 MeV, 5000 ns
Peak Dose Rate	10^{11} Rads/sec (in Silicon)	n/a
Neutron Production	n/a	4×10^{13} neutrons/sec

3.1.2. Water-Cooled Aluminum Output Window

Many of the current uses of the RPI LINAC use a brute-force technique for producing large neutron or gamma ray flux at high electron beam current. A robust, durable output window is needed for such environments where window survivability is critical, and electron beam scattering and bremsstrahlung production are a lesser concern. The existing output window is made of two 1/32" thick, aluminum sheets separated by a 1/16" thick gap of circulating water. Monte-Carlo techniques are used to assess this window's effect on electron beam scattering and bremsstrahlung production. Figures 36-37 show the results from MCNP-4C2 [9] simulations for the electron and photon angular distribution at the exit surface of the output window. Appendix F shows the MCNP input file. The simulation results in the electron and photon distribution as a function of the cosine of the exit angle. The output is manipulated to determine the exit angle, and through symmetry arguments, the output for positive exit angles is used for negative exit

angles. This is shown as data points in Figures 36-37, and the solid lines are the gaussian fit of the data points. The fitting function uses the following definition for the gaussian; y_0 is the baseline amplitude, A is the area under the curve, x_0 is the centroid of the peak, and w is two standard deviations (2σ) [46].

$$y = y_0 + \frac{A}{w\sqrt{\frac{\pi}{2}}} e^{-\frac{2(x-x_0)^2}{w^2}} \quad (57)$$

Figure 36- Electron beam divergence simulated for the water-cooled output window using 60 MeV electrons. MCNP results were fit to a gaussian distribution, with $2\sigma=63$ mrad.

Figure 37- Photon beam distribution simulated for the water-cooled output window using 60 MeV electrons. MCNP results were fit to a gaussian distribution, with $2\sigma=52$ mrad.

The primary problem with the water-cooled output window rests with its impact on the electron beam divergence. Consider the analysis of the electron beam divergence effects on the PXR photon distribution in Section 2.3.6 . The larger electron beam divergence flattens the photon distribution. In a small detector solid angle, this effect results in less photon flux at the detector. For 60 MeV electrons, θ_{ph} is 8.5 mrad and the MCNP-calculated electron beam divergence is about 31.5 mrad or nearly $4\theta_{ph}$. So the severity of the PXR broadening shown in Figure 33 is small compared to what would occur with use of the water-cooled output window. The calculated bremsstrahlung with energy between 1 keV and 60 MeV produced from this output window is 7.3×10^{-3} photons/electron. The photon angular distribution is shown in Figures 37. This relatively large quantity of bremsstrahlung is incident on the PXR crystal, and it may cause unwanted Compton scattered photons or crystal-diffracted photons at the PXR detector location. For these reasons, a new output window was designed for the PXR experiments.

3.1.3. Beryllium Output Window

The window to replace the water-cooled window needed to have minimal impact on the electron beam and to produce as little bremsstrahlung as possible. Beryllium (Be) was the logical choice because of its low atomic number ($Z=4$) and because of its common use in particle accelerators [47], in X-ray detector windows [48], and in vacuum systems [49]. Some other materials were compared to Be. Figure 38 shows the calculated 100 KeV bremsstrahlung yield [photon/s/steradian] produced at 20° away from the electron direction using the analytical expression in Equation 11. For the calculation, the electron energy is 60 MeV, and an electron current is 25 nA. Obviously, thinner windows produce less bremsstrahlung. In the case of 100 keV photons, Be is superior to the other materials for all thickness.

Figure 38- Photon beam distribution simulated for different output window materials using 60 MeV electrons.

There are some structural constraints on the Be thickness allowed for low pressure vacuum systems. The 10-mil (250 μ m) thickness was the thinnest that could be warranted for used with the RPI LINAC [50]. The Be window was supplied by K-Tek International, Inc with the following specifications: Be purity: 98.5%; Be thickness 0.25 ± 0.03 mm; MDC 3-3/8" flange; Be aperture diameter 33 ± 0.2 mm. The MCNP

techniques used to calculate the electron and photon angular distribution for the water-cooled window are not as appropriate with this thin Be window. The Be has so little impact that MCNP does not have the angular resolution to examine these parameters as well. Figure 39 shows the complications in attempting such a calculation of the electron beam divergence.

Figure 39- Photon beam distribution simulated for the 10-mil Be output window using 60 MeV electrons. MCNP results were fit to a gaussian distribution, with $2\sigma=4$ mrad.

As a comparison, the electron beam divergence for 2σ is calculated using Equation 13. The analytical result for 10-mil Be is 5 mrad compared to 4 mrad simulated with MCNP. Of the other materials considered for the window, a 10-mil thickness results in an electron beam divergence 2σ of 12 mrad (Al), 19 mrad (Ti), 66 mrad (Ta), and 72 mrad (W). In any event, the impact on the electron beam divergence is substantially reduced using the Be window.

The other improvement with the use of the Be window is in total bremsstrahlung production. Less bremsstrahlung is produced from the Be window. Figure 40 compares the spectrum of total bremsstrahlung produced in the forward direction from the 10-mil Be window and from the water-cooled aluminum window as a function of X-ray energy. The same Monte-Carlo simulation parameters are used to determine the bremsstrahlung

exiting from the window. At low energies <8 keV, the Be window produces more bremsstrahlung than the water-cooled window at these energies. The water-cooled window produces more bremsstrahlung photons in this energy region, but self-absorption attenuates these photons along the exit path from the window material. For energies >8 keV, the bremsstrahlung from the aluminum window increases to a peak value near 25 keV, then begins to decrease characteristically with energy (E^2). For energies >25 keV, the bremsstrahlung from both the windows are decreasing at nearly the same rate with the intensity from the aluminum window about a factor of ten greater than the Be window.

Figure 40- MCNP simulated forward bremsstrahlung produced from the water-cooled aluminum window and the 10-mil Be window interacting with 60 MeV electrons.

3.2 ADDITIONAL ELECTRON MONITORING

During PXR experiments, other systems are added to measure the electron beam current and to monitor the electron beam position. Because the PXR production is per electron, it is necessary to accurately measure the electron beam current in order to make comparisons with theory. Electron beam monitoring is necessary to insure that the electron beam is aligned and focused on the crystal so that the LINAC current measurement represents the electron beam current incident on the crystal

3.2.1. Beam Charge Monitor (BCM)

Although the lead backstop is appropriate for monitoring current during LINAC tuning, this is problematic during PXR experiments because the generation of neutrons and gamma rays can damage the PXR detection system. Instead, a Beam Charge Monitor (BCM) is used to directly measure the electron beam charge without affecting the electron momentum. This is done through induction of current in a solenoid coil with its long axis aligned with and centered on the electron beam path. A Bergoz BCM is permanently mounted on the Be window drift pipe. Figure 41 shows the BCM photographed from the side of the LINAC. At the left is the coupling between the LINAC and the modified Be Window assembly. Notice that the transition in drift pipe size, from diameter of 4" to 2". The electron beam direction is left to right, and the BCM is mounted concentrically on the 2" diameter drift pipe. Lead shielding with 2" thickness surrounds the drift pipe just before and just after the BCM.

Figure 41- Photograph of the BCM and the coupling of the Be window assembly to the LINAC.

With locally adapted software [51], the Bergoz BCM measures the mean charge per LINAC pulse averaged over a several hundred LINAC pulses. For PXR experiments,

the LINAC repetition rate is 400 Hz. The electron beam current is determined from the BCM output and the repetition rate. The BCM must be calibrated, and this is done with the lead backstop using electron beam currents from 50 nA to a few μA .

3.2.2. Beam Position from Optical Transition Radiation (OTR)

As discussed in Section 2.2.4.1 transition radiation is emitted with a wide range of photon frequencies, including visible light. This fact offers the ability to image the electron beam position on a target crystal using a video camera. The light is most easily observed in the backward geometry in order to avoid detection along the electron path and the forward dominated bremsstrahlung. A hollow cone of TR would be emitted from the interaction of the a pencil beam of electron with the crystal. However, the larger electron spot size from the RPI LINAC generally broadens the OTR into a gaussian beam reflected from the crystal surface with directionality approximated by γ^{-1} . The general set-up for OTR beam monitor is shown below in Figure 42. The PXR crystal is used to generate the OTR. The crystal is placed at 45° to the electron beam, and the mirror is placed at 90° to the electron beam. A well-shielded video camera views the OTR reflected from the mirror, and the output is sent to a distant TV monitor in the LINAC control room. Two camera systems were used: a Samsung SCC-340 N low illumination color camera and a Panasonic WV-200 analogue black and white camera. In most cases, the analogue camera is used to avoid radiation damage to the digital camera. Some options are available for saving the OTR images. The camera output can be fed through a VCR for recording analogue information. The other alternative is to send the camera output to a personal computer (PC) which has a Piccolo digitizing card for recording digital still images or sequenced short movies. Photolite software, version 3.0, is used for OTR digital recording.

Figure 42- Top view of the general set-up for monitoring the electron beam position on the PXR crystal. Signal is sent to the LINAC control room.

The investigation of OTR is another project of its own. In this research, the OTR is not studied in detail. Rather, the mechanism is simply used as a tool to verify that the electron beam is generally centered on the crystal. The positions of the OTR monitoring system's mirror and camera are roughly aligned. Because the backward OTR is highly directional, it is typically necessary to rotate the crystal slightly about the 45° angle in order to observe the OTR at the camera. An intense beam of visible light can be observed when the system is properly aligned. At crystal angles slightly misaligned, the OTR can appear to originate from an edge of the crystal with slightly reduced intensity. This can be misleading information for the LINAC technician attempting to focus the electron beam and to steer the electron beam onto the center of the crystal. Consequently, it is necessary to properly align the OTR system by rotating the crystal before any repositioning of the electron beam.

Two additional qualitative observations are raised. First, with the opaque crystals such as Si, it is assumed that there is no diffusion of light in the crystal, and the size of the observed OTR spot reflects the size of the electron beam on the crystal. In these crystals, the forward OTR is not observable from the configuration of Figure 42, and at low beam currents the backward OTR has a distinct blue color. Figure 43 shows the OTR from the Si crystal while the LINAC was at high electron beam current ($\sim 1 \mu\text{A}$) during machine tuning. Second, with semi-transparent crystals, the component of the forward OTR can be observed when the crystal is not placed near the 45° angle. In fact, with a LiF crystal in the Bragg geometry and small θ_B , the OTR appears as a streak of blue light depicting the electron path across the crystal. This is likely forward OTR that has been internally scattered in the crystal. This is shown in Figure 44, in which $\theta_B = 15^\circ$, and the surface is just 15° from the electron beam direction. Note that in this case the camera is on the opposite side of the LINAC. In this view of forward OTR, the crystal thickness (1.5 mm) is much smaller than the diameter of the electron spot size (1-2 cm), and images sequenced over time demonstrate variations in the intensity and uniformity of the streak of light. Because the camera readout time $1/60$ s long compared to the time between pulses (250 ms), this observation suggests that the electron beam may wobble or drift back and forth over time.

Figure 43- Backward OTR observed from Si with surface 45° to the electron beam direction.

Figure 44- Forward OTR observed from LiF with surface 15° to the electron beam direction.

3.3 CRYSTALS AND ALIGNMENT

A list of crystals acquired for RPI PXR experiments is shown in Table 17 in order of the material atomic number, Z. Information includes the crystal surface normal vector $\langle hkl \rangle$, surface dimensions, thickness, supplier, and any general comments are added, such as mosaicity or flat information. SPI-1, 2, 3 refer to graphite mosaicity with values $0.4^\circ \pm 0.1^\circ$, $0.8^\circ \pm 0.2^\circ$, and $3.5^\circ \pm 1.5^\circ$, respectively.

3.3.1. PXR Target Crystals

Table 17. Inventory of crystals acquired for the RPI PXR experiments.

<i>Material</i>	<i>Surface</i>	<i>Dimension</i>	<i>Thickness</i>	<i>Supplier</i>	<i>Comments</i>
HOPG	$\langle 001 \rangle$	10 x10 mm	1 mm	Alfa Aesar	SPI-1
HOPG	$\langle 001 \rangle$	10 x10 mm	2 mm	SPI	SPI-2
HOPG	$\langle 001 \rangle$	20 x20 mm	2 mm	SPI	SPI-3
LiF	$\langle 100 \rangle$	10 x10 mm	1 mm	MTI	
LiF	$\langle 100 \rangle$	D=50 mm	1.5 mm	MTI	$\langle 110 \rangle$ flat
Si	$\langle 111 \rangle$	D=50 mm	500 μm	Virginia	
Si	$\langle 100 \rangle$	D=50 mm	500 μm	Virginia	$\langle 110 \rangle$ flat
Si	$\langle 100 \rangle$	D=50 mm	300 μm	Virginia	$\langle 110 \rangle$ flat
Si	$\langle 100 \rangle$	D=50 mm	279 μm	Virginia	$\langle 110 \rangle$ flat
Si	$\langle 100 \rangle$	D=50 mm	90 μm	Virginia	$\langle 110 \rangle$ flat
Ge	$\langle 111 \rangle$	D=50 mm	500 μm	University	
Ge	$\langle 111 \rangle$	D=50 mm	500 μm	MTI	
Cu	$\langle 111 \rangle$	D=10 mm	1 mm	MaTeck	
W	$\langle 111 \rangle$	D=10 mm	1 mm	MaTeck	

3.3.1. Goniometer

The crystal is moved by a Huber three-concentric axis, goniometer with angular resolution of 0.001° supplied with control software by Crystallogic, Inc. A drawing of the goniometer is shown in Figure 45 [52].

Figure 45- Drawing of Huber three-axis goniometer with center of rotation 11.0 cm above the top plate.

The goniometer software has three angles for crystal movement: Ω , α , and β . Ω is the rotation angle around a vertical axis, and both α and β are tilt angles. By convention, the crystal position for $\Omega=\alpha=\beta=0$ is when the crystal large face is parallel to the electron beam direction, and there is no tilt. Using this convention, α serves to tilt the crystal face up and down, while β serves to rock the crystal laterally across the electron beam. The range of motion limits for Ω is $\pm 180^\circ$ and for α, β is $\pm 15^\circ$. The goniometer is controlled remotely from a PC.

The goniometer is positioned on a mobile, elevating table modified with aluminum I-beams that raise the goniometer center axis to the electron beam height approximately 61.5" above the floor of the LINAC target room. Figure 46 shows the

goniometer table, I-beams, goniometer, and a LiF crystal held in front of the Be output window.

Figure 46- Photograph of the goniometer table positioned in front of the Be output window. A 2" diameter LiF crystal is held in an optical mount.

Notice that besides the 0.5" aluminum platform that partially covers its top, the goniometer is effectively unshielded from any electron interactions occurring at the window or at the crystal. Except for the motor that drives the Ω rotation, the other two motors are totally exposed in order to allow freedom of motion. The only shielding offered to the goniometer is a 2" wall of lead to shield any radiation moving below the drift pipe. At typical electron beam currents $<1\mu\text{A}$, no detectable activation has occurred with the goniometer, and there has been no degradation of its performance after nearly three years of service.

3.3.2. Crystal Holders

The absence of activation in the goniometer is not always the case with the crystal holders. The crystal holders are black anodized aluminum (Part #L54-996) with stainless steel posts (Part #L36-495) held in post holder (Part L03-646) all supplied by Edmund Industrial Optics. For the larger, 2" diameter crystals care is taken to position the electron beam far from the holder, near the upper half of the crystal. Even with the OTR to monitor the electron beam, this precaution is not always sufficient. Figure 47 shows a picture of the electron beam effects on a new LiF crystal never exposed to the LINAC electrons. The crystal is darkened by the electron interactions. At the lower right part of the crystal is the unintended reflection from an overhead light, which should be disregarded. However, at the lower center part of the crystal along the flat, there are two clear circular regions that exactly match the position of the two thumbscrews for the aluminum mount. The thumbscrews can be seen in the photograph of the aluminum holder shown on the right in Figure 48. This observation makes clear the fact that the holder is struck by electrons or possibly bremsstrahlung moving along the path of the electrons.

Figure 47- Photograph of the 2" diameter LiF crystal with apparent darkening from electron beam interactions and obvious shielding from optical mount thumbscrews.

Electron interaction with the crystal holder material is a possible source of noise during PXR detection. A remedy to this problem is to either suspend the crystal remotely so that little material is in the electron beam or to use a low density, low Z material to hold the crystal. The later option is done by cutting customized crystal holders from styrofoam poster board. The crystal is held in compression in gaps cut into the poster board. This technique is needed for the small 10 mm x10 mm crystals. For the larger crystals it reduces the impact of electron interaction with the mount. The disadvantage is that the poster board is less mechanically stable and suffers from the potential of vibration caused by future forced-air cooling. Figure 48 shows the styrofoam holder and the aluminum holder.

Figure 48- Photograph of the styrofoam poster board mount (left) and the anodized aluminum optical mount (right).

3.3.3. Alignment to the LINAC

The LINAC output window is changed before each series of PXR experiments (runs). The goniometer table is mobile, and it must be properly positioned at the beginning of each series of PXR run. A laser technique is used to place the center of

mass of the crystal mount post at the center of the Be output window and to align the $\Omega=0$ angle with the direction of the electron beam. A laser level with a horizontal line is readily available at most hardware or home improvement stores. Before placement of the goniometer table, the laser level is positioned on its side on a level surface downrange of the Be window and near the end of the LINAC target room. The horizontal level line is now vertical. With some alignment, this vertical laser line is directed back towards and centered on the Be window. The laser line is also centered on the drift tube at a distant point near the bending magnet, M2. A 500 μm silicon crystal is held in the goniometer at $\Omega=\alpha=\beta=0$. The goniometer is centered on the mobile table. A vertical post held by the goniometer and the vertical center of the goniometer table serve as reference point for centering the table on the output window. These marks are aligned with the laser through translation of the goniometer table left or right. Once the laser is on the Si crystal, the table is rotated until the laser diffraction from the crystal is symmetric on the Be window. This is an iterative process between translating the table and rotating the table. The result is that the goniometer angle $\Omega=0$ is aligned with the electron beam direction and the center of mass of the crystal mount post is centered on the Be window.

3.4 DETECTION SYSTEMS

Four detectors are used during the RPI PXR experiments: a cadmium zinc tellurium (CZT) X-ray detector, a silicon (Si) X-ray detector, and a bismuth germanate (BGO) gamma detector, and an intensified CCD camera with a gadolinium oxysulfide (GOS) scintillator. The X-ray detector used for most of the PXR experiments is a 500- μm thick Si Amptek XR-100CR detector with 25 mm^2 area, 20 μs pulse shaping, and a resolution of 350 eV at 17.5 keV. A 2 mm thick CZT Amptek XR-100T-CZT detector with 9 mm^2 area and resolution of 1.5keV at 122 keV was tested, but its poor resolution in the PXR energies 10-30 keV convinced us that the Si detector was best for PXR X-ray spectroscopy.

3.4.1. Silicon X-ray Detector Efficiency

The silicon detector has a 1 mil Be window (x_{Be}) and a Si thickness of 500 μm (x_{Si}). The intrinsic photo-peak efficiency, $\epsilon(E)$, for the silicon detector can be calculated

using the following expression. ρ is the mass density, μ is the total mass attenuation coefficient, and subscripts *Be* and *Si* are for beryllium and silicon, respectively. $\mu_{Si(PE)}$ is the photon-electric linear attenuation coefficient. The peak efficiency for this detector occurs at 8 keV with a value of 0.994.

$$\varepsilon(E) = e^{-\mu_{Be} x_{Be} \rho_{Be}} \left(1 - e^{-\mu_{Si} x_{Si} \rho_{Si}} \right) \frac{\mu_{Si(PE)}}{\mu_{Si}} \quad (58)$$

Figure 49- Calculated Si detector photo peak efficiency as a function of X-ray energy ($x_{Be}= 25 \mu\text{m}$, $x_{Si}=500 \mu\text{m}$).

3.4.2. Silicon X-ray Detector Calibration

Energy calibration for all of the X-ray detectors is done with the $K_{\alpha 1}$ florescent lines of Zn (8.64 keV), Zr (15.77 keV), and Sn (25.27 keV). Calibration is done with the detector in the target room. Although the LINAC is not operating, all other conditions are identical to the PXR experiment. To excite the material $K_{\alpha 1}$ emission, a well-collimated ^{241}Am (59.5 keV) source with activity of 1mCi is directed towards a 1 mm slab of one of the three materials. The Si detector is placed in a backscattered geometry so as to minimize any detection of the ^{241}Am source. Spectra are collected for 2 minutes. The Amptec MCA software is used to identify the centroid of the respective $K_{\alpha 1}$ peaks, and those energies are used in a linear energy calibration. Once this calibration is done, a more expedient check of the detector operations and calibration is done with a ^{57}Co

calibration source with X-ray emission at 6.4 keV and 14.4 keV. There was some suspicion that the LINAC RF may alter the calibration. To test this, a ^{133}Ba calibration source with X-ray energies of 31 keV and 35 keV was inserted with the detector while PXR spectra were taken. No shift in energy calibration was observed.

3.4.3. Silicon Detector Data Acquisition

The Si Amptek XR-100CR detector power supply is well shielded in the target room at a height about 30" below the electron beam height during PXR experiments. The power supply has a built-in amplifier, which is set to a value of 2.2 and a rise time discriminator (RTD), which is active for PXR experiments. The RTD rejects pulses that do not have the "good" shape of an X-ray event. The RF environment of the target room can disrupt X-ray spectroscopy. Detector cables leading out of the target room to the multi-channel analyzer (MCA) can act like antennae. To insulate from this effect, the X-ray detector cable is encased in copper tubing. The length of the cable is between 75-100 feet. To prevent from signal ringing, the cable end has 50-ohm termination through either instrumentation or an added resistor. The signal leads to a portable, Eagle Classic Amptec-NRC MCA (now supported by Canaberra). The MCA settings allow for X-ray detection from 1.4 keV to 28.9 keV with nominal 1024 channels. Settings are listed in Appendix G. The MCA can gate the signal detection. This allows for detection of events only associated with the LINAC pulse. After some of the early PXR experiments, we discovered that the background between LINAC pulses is very low and a gated and ungated spectral are identical.

3.4.4. Silicon X-ray Detector Shielding

The silicon detector housing has the dimensions shown in Figure 50 [48]. Its dimensions are the basis for building the detector shielding used for the Si, CZT, and BGO detectors. The Si and CZT detectors have identical housing dimensions.

XR-100CR Mechanical Dimensions

Figure 50- Mechanical dimensions for the Si and CZT X-ray detectors.

The detectors are heavily shielded with lead. An aluminum box was made to support the lead surrounding the detector so that the detector could slide in and out of the box without disrupting the shielding. Several aluminum plates are made to slide snugly in and out of the box. The plates are used for detectors and for the laser used for detector/collimation alignment. While the box is stacked with lead, the detectors or laser can be installed or removed. A 5-cm thick lead brick is attached to the side of the detector box facing the PXR crystal. A circular hole is drilled in the brick so that the detector collar (1.8 cm diameter) slides entirely into the brick. Figure 51 shows a photograph of the detector box and the attached lead brick with the drilled opening.

Figure 51- Detector aluminum housing with attached lead brick and 0.7" diameter opening.

Similarly, the alignment laser head slides into the brick so that the laser emission location coincides with the center of the detector face. Figure 52 shows the Si detector and the alignment laser mounted on their aluminum plates. The position of the detector is based on the experimental design. The Bragg angle determines the detector angle, $\Omega=2\theta_B$. Two different X-ray collimators are used. These were made by milling-out a square groove from the long face of a lead brick. Stacking another lead brick on top of the milled brick completes the collimation. The small collimation has dimensions of 3 mm x 3 mm. The large collimation, used only during imaging experiments, has dimensions of 1.6 cm x 1.6 cm. A series of steps using the alignment laser inside the detector box is used to position the detector face at the appropriate Ω angle at a distance of 274 cm (9') from the PXR crystal. The alignment process takes advantage of the mirror surface of the crystal and the goniometer motion. In the end, the detector and the X-ray collimation is aligned with respects to the PXR crystal and the LINAC output window. The alignment process is explained in Appendix H.

Figure 52- A photograph of the laser used for detector alignment (at left) and Si X-ray detector (at right). Both are mounted on aluminum bases that slide in and out of the detector housing.

The typical lead shielding for the detectors includes 52 lead bricks each with dimensions 5 cm x 10 cm x 20 cm (2"x4"x8") weighing approximately 10.9 kg (24lbs) each. The total weight of the lead shield is about 568 kg (1250 lbs). A aluminum-wheeled, four post mechanical elevating table (Vestil Manufacturing Corporation, Model MT 3042-HP) with lifting capacity of 909 kg (2000 lbs) is used to support the detector and shielding. A top view of the shielding scheme is shown in Figure 53. The gray rectangular sections represent the lead bricks, and the white spaces represent air and the X-ray collimation. The lead shielding thickness from the front X-ray entrance to the detector face is approximately 46 cm (18").

Figure 53- Typical detector lead shielding and collimation. This includes 52 lead bricks and approximately 46 cm of X-ray collimation.

3.4.5. Other Detectors

The three other detectors are discussed briefly because they are not the primary detectors for this work. Their general characteristics such as dimension, resolution, and X-ray intrinsic efficiency are presented. Equation 58 is used to calculate the theoretical detector intrinsic efficiency. Plots extending to energies where the efficiency drops to 0.01 are shown for each detector. When data are collected using one of these detectors, any additional characteristics needed for data analysis will be added in the results chapter.

3.4.5.1. CZT Detector

The CZT detector is Amptek Model XR-100T-CZT. It has the same housing as the Si detector, but the Be window is 10 mil (250 μm) thick. The active area is 9 mm^2 , and the CZT crystal is 2 mm thick. The composition of the CZT is $\text{Cd}_{(1-x)}\text{Zn}_x\text{Te}$ [53], and the weight fractions used for calculating the linear absorption coefficient are 0.45 for Cd, 0.05 for Zn, and 0.5 for Te. MeuDAt [16] is used to determine μ_{CZT} , and the CZT density is 7.19 g/cm^3 . The resolution is 1.5 keV FWHM at 122 keV. Figure 54 shows the calculated intrinsic photoelectric efficiency for the CZT detector.

Figure 54- Calculated CZT detector intrinsic photoelectric efficiency. Window is 10-mil Be and the detector is 2 mm CZT.

3.4.5.2. BGO Detector

The Bismuth Germanium Oxide ($\text{Bi}_4\text{Ge}_3\text{O}_{12}$) detector was assembled locally with a 0.75" diameter BGO scintillator with a thickness of 1 cm. The scintillator was coupled to a 0.75" diameter Photonis photo multiplier tube (Model XP1921) with Photonis voltage divider base (VD308). The operating voltage is +900-1000V. Lanco International, Inc., the Photonis U.S. distributor, supplied the scintillator and photo multiplier tube. The assembled detector is sealed for light then mounted on an aluminum detector plate for use with the Si detector box. The BGO density is 7.13 g/cm^3 . Figure 55 shows the calculated intrinsic photoelectric efficiency for the BGO detector. The measured energy resolution has a FWHM of 18% at 511 keV.

Figure 55- Calculated BGO detector intrinsic photoelectric efficiency. The detector is 1 cm BGO with no window.

3.4.5.3. Intensified CCD Camera

The CCD Camera is a 50 mm X-ray Gemstar System manufactured by Photonic Science. The active size of the CCD (charge coupled device) is 40 mm x 30 mm. The pixel resolution is 1392x1040 (4:3 aspect ratio) leading to an effective pixel size of $28 \mu\text{m} \times 28 \mu\text{m}$. The scintillator is Gadolinium Oxysulphide ($\text{Gd}_2\text{O}_2\text{S}$) with 15 mg/cm^2 surface mass density. This CCD camera has on-chip binning capabilities and a 12 bit

grayscale (4096 levels). The peak scintillator efficiency is at about 15.5 keV, and there is a jump at the absorption edge at 50.3 keV. Figure 56 shows the calculated intrinsic photoelectric efficiency for the GOS scintillator.

Figure 56- Calculated GOS scintillator CCD detector intrinsic photoelectric efficiency. The window is 10-mil Al, and the scintillator has surface density of 15 mg/cm².

3.5 Experimental and Electronic Set-up.

Figure 57 shows the typical PXR experimental set-up. Variations in the experiments arise in changes in the Bragg Angle θ_B which changes the location of the detector. Additionally, if the experiment involves imaging, then the large collimator is used and the crystal must be displaced further from the output window so that the collimator prevents direct line-of sight of the window. A geometric calculation for the necessary window-crystal distance is done as a function of θ_B and the collimator width. This is shown in Appendix I.

Figure 58 shows the typical PXR electronics configuration. At the left are the inputs and outputs to the LINAC target room. Two personal computers (PC) are used for data acquisition and motion control. Computer 1 is used for X-ray spectroscopy and goniometer control. Computer 2 is used for CCD imaging and control of other less frequently used motorized devices such as a rotation stage and a translations stage.

Figure 57- Typical PXR experimental set-up. Shown here is LiF (220) in Laue geometry with $\theta_B = 15^\circ$.

Figure 58- Wire diagram for data acquisition and motion control.

CHAPTER 4

RESULTS AND ANALYSIS

The results are organized functionally by experimental goal and generally appear in chronological order. Approximately 60 hours of LINAC operating hours were used to collect this data over a period of three years. Some experiments were more successful than others. This chapter does not include the results from all of the RPI PXR experiments. The chapter is devoted to the milestone experiments from which new scientific challenges were met or new scientific information was gathered. A variation of the typical experimental set up seen in Figure 57 is used with some specific θ_B . For each experiments, a table describes a general set of parameters for the experiment to include the Bragg angle (θ_B), crystal size, the predicted 1st-order PXR energy, the electron energy, the electron beam current, comments, the LINAC window, and the experiment date. Each experiment has two sections: *DATA ANALYSIS*, which is presented in tables and graphs to interpret the results, and *CONCLUSIONS*, which draws conclusions from the results.

Prior to discussion of the results, there are some routine procedures that occur when collecting and interpreting data. This first section of this chapter is the Analysis Methods. These include corrections to measured count rate due to detector deadtime, detector efficiency, and photon attenuation in air. Additionally, measuring the rocking curve and comparing the spectra with the predicted energies for PXR and diffracted bremsstrahlung helps to characterize the source of the measured spectra.

4.1. Analytical Methods.

4.1.1. Assessment of Diffracted Bremsstrahlung.

It is likely that the electron beam is accompanied by bremsstrahlung produced from electron interactions with parts of the LINAC to include areas around the bending magnets, transitions between drift pipes and flanges with different sizes, and mostly the output window. These photons are subsequently referred to as Diffracted Bremsstrahlung Radiation (DBR). This bremsstrahlung can be diffracted to the detector location with the same energy as PXR when the Bragg condition is satisfied. However, with rotation of

the crystal about the Bragg angle, θ_B , the energies of the PXR and of the DBR start to diverge. The energy for DBR is calculated using following equation [54].

$$E_{DBR} = \frac{c\hbar|\vec{\tau}|^2}{2\sqrt{\epsilon_0}\vec{\tau} \cdot \hat{\Omega}} \quad (59)$$

Again, $E_{PXR}=E_{DBR}$ when the Bragg condition is satisfied, $2\phi=\Omega$. Figure 59 shows both X-ray energies for a LiF(220) Laue geometry with θ_B near 15° and a detector location at 30° from the electron beam direction, ($\Omega=30^\circ$). Rotating the crystal causes variation in the incident angle, ϕ . At incident angles far from 15° , the PXR remains linear with changes in ϕ , but the DBR has a distinct curvature that diverges to higher energies than the PXR energy.

Figure 59- Comparison of PXR and DBR energies from LiF(220) with θ_B near 15° and the detector fixed at $\Omega=30^\circ$.

4.1.2. Deadtime Correction.

In every measured PXR spectrum, there is the need to correct the measured count rates for detector deadtime and pile-up. During this investigation of PXR, a model for deadtime correction was developed for pulsed spectroscopy [55]. Because of the Si detector's 20 μ s resolving time and the ADC conversion time, the detector can measure just one photon event per LINAC pulse. This model is based on Poisson statistics and

the random arrival of one of two types of photons: PXR and bremsstrahlung photons. In particular, four calculations are made to correct the count rate in the first-order peak (n_1), in the second-order peak (n_2), the pile-up of two first-order photons counted in the second order (p_1), and the total count rate (n_t). These four quantities can be calculated from three measured quantities in the measured spectrum: (r_1) the measured count rate in the first order peak, (r_2) the measured count rate in the second order peak, and (r_t) the measured total count rate in the first order peak. The RPI LINAC pulse rate, f , for these experiments is typically 400 Hz. The expressions for calculating the four quantities are shown below.

$$n_1 = \frac{fr_1}{f - r_t} \quad (60)$$

$$n_2 = \frac{fr_2}{f - r_t} - \frac{f}{2} \left(\frac{r_1}{f - r_t} \right)^2 \quad (61)$$

$$p_1 = \frac{f}{2} \left(\frac{r_1}{f - r_t} \right)^2 \quad (62)$$

$$n_t = f \cdot \ln \left(\frac{f}{f - r_t} \right) \quad (63)$$

Note that in Equation 61 the second term is the contribution of two first-order photons counted as one second-order photon in the second-order peak. Consequently, this second terms is also the incidence of first-order pileup, p_1 . The deadtime correction is used primarily as a tool to determine the real photon rates at the detector so that comparisons can be made with predicted PXR photon yields. The first validation of the model was to observe linear increases in the deadtime corrected count rates with increasing electron beam current when the measured count rates typically reach some saturation point at high electron beam currents. However, in the course of our experimental investigations, other data were collected that further supports the deadtime correction model. These experiments will be discussed as a separate section at the end of this chapter.

4.1.3. Corrections for Air and Detector Efficiency.

Corrections for detector efficiency and attenuation in air must be done to make comparisons between measured and predicted PXR yields. The detector efficiency was

discussed early in Chapter 3. The pathway from the crystal is typically $x=274$ cm, and so the transmission (T) through this pathway can be calculated using the total linear attenuation coefficient in air, μ_{air} , where $T=e^{-\mu_{\text{air}}x}$. Figure 60 shows the air transmission and the detector efficiency plotted together so that their relative values can be observed. Often times these effects move in opposite directions. When the detector efficiency is at its peak near 8 keV, there is effectively no transmission, and as the energy rises so that there is transmission, the detector efficiency is beginning its decline.

Figure 60- Si detector intrinsic efficiency and X-ray transmission through a 274 cm air pathway.

So as we begin to examine the PXR experiments, there is often an examination to verify that the measured spectrum is not contaminated with DBR. With the water-cooled aluminum output window, the spectrum does have DBR, but we will demonstrate that with the 10-mil Be window there is no evidence of DBR in the measured spectra. When data are compared to theoretical yields, the deadtime correction is applied and additional corrections are made for detection efficiency and air attenuation.

4.1.4. Detector Saturation Peak.

In the spectra collected using the Si detector, the typical MCA settings use 1024 channels with energy binning up to 39 keV. Measured photons with energies greater than 39 keV are all placed in the last bin of the MCA. When viewing the measured spectra, one should remain aware of this procedure. Routinely, there is a peak in the X-ray spectra at the last channel of the MCA. This peak is referred as the "Saturation Peak", and it represents the binning of measured photons with energies greater than 39 keV. This does not represent a large count rate of 39 keV photons. The source of the saturation peak photons is discussed later in the Results Chapter.

4.2 Early Experiment with the water-cooled window.

These early experiments were done with the BCM externally positioned on the exit side of the aluminum water-cooled output window. There was no use of OTR beam monitoring. In the early experiments, the measures to control the experimental parameters needed some refinement. Consequently, many of the conclusions from these early experiments are more qualitative than quantitative with the aim of deciding strategies to improve the execution of subsequent PXR experiments.

4.2.1. RPI's first observation of PXR

While there were earlier, unsuccessful attempts, the first observation of PXR at RPI occurred on 9 May 2002 using a silicon crystal. The general experimental parameters are tabulated below. In order to use the Si(220) diffraction planes, the wafer flat was rotated 45° from the horizontal so that the planes used for this experiment form a 45° with the surface of the wafer, the *Asymmetric Laue geometry*.

Bragg Angle	30°
Crystal	Si (220), <i>Asymmetric Laue</i> D= 50mm, t=500 μm
Predicted Photon Energy	6.45 keV
Electron Energy	50 MeV
Current	448 nA
Comments	Flat at 45°
Linac Window	Al Water Cooled
Date	9 May 2002

In this experiment, coincidence counting was used to detect events occurring around the LINAC pulse, and a ^{57}Co calibration source was inserted with the detector to assess the LINAC effects on energy calibration and detector deadtime. The detection gating window width was 70 μs triggered by the LINAC's 1 μs pulse. Since the repetition rate was 400 Hz, there is one pulse per 250 ms, in which the detector is on for just a fraction (2.8×10^{-4}) of the time. For some of the spectra, the ^{57}Co was placed in line with the collimation about a cm from the detector face. Prior to employing the Be window, the BCM was an independent device, free to be positioned at my discretion. In these early experiments, the BCM was positioned at the exit side of the aluminum water-cooled output window. Because of the 6" length of the BCM, the crystal was a total distance of 11.75" from the output window. The crystal was held in the optical mount with the flat rotated approximately 45° to the horizontal (*Asymmetric Laue* geometry).

4.2.1.1. Data Analysis

Table 18 shows the detector response to the ^{57}Co with and without electron beam conditions with no crystal in the mount. The net count rates (cps) are shown for the 6.4 keV peak, the saturation peak, and the spectrum total. In this case, the saturation peak is where all photons with energy >29.9 keV are binned. Different LINAC conditions are compared, and the results with and without detector gating are shown. Note that in this first experiment, the multi-channel analyzer (MCA) was set for 2048 channels.

Table 18. Detector ^{57}Co count rates for various LINAC conditions with no PXR crystal.

<i>Condition</i>	<i>6.4 keV</i>	<i>Sat</i>	<i>Total</i>
No Beam	90.2 cps	3.3 cps	158 cps
RF Only	91.3 cps	3.3 cps	163 cps
Beam			
No Crystal	91.7 cps	9.3 cps	173 cps
Gate Beam			
No Crystal	0.4 cps	3.5 cps	11 cps

Figure 61 shows the two spectra of Si (220) PXR with the ^{57}Co (lower plot) and without the ^{57}Co (upper plot). Figure 61 is shown to address two issues. First, large

Bragg angles can result in a low PXR energy and large photon attenuation along the air pathway to the detector. The 60° detection angle was used to avoid electron and high-energy bremsstrahlung detection. But the consequence of this relatively large Ω angle is a Si (220) PXR photon energy that is heavily attenuated along the air pathway to the detector. In this case, the distance was approximately 9'3" (~282 cm) through which the 6.7 keV PXR is attenuated by more than three orders of magnitude. The first measured peak is at 13.4 keV, Si (440), and the next peak near a multiple of the first order energy is at 19.8 keV, Si (660). Second, the LINAC RF and electron beam do not affect the detector energy calibration. Despite some concern that energy calibration may be affected by conditions in the LINAC target room, the energies for the ^{57}Co X-ray peaks remained unchanged, as seen in the lower plot of Figure 61.

Figure 61- Two plots of Si (220) at $\theta_B=30^\circ$ taken with detector gating. Lower plot is with the ^{57}Co , and the upper is without the ^{57}Co . Electron beam current is 448 nA.

4.2.1.2. Conclusions

Although this is the first experiment with relatively poor results, some conclusions can be drawn. Table 18 demonstrates that the detector shielding with the

narrow collimation (3mm x 3mm) sufficiently shields the detector from RF and electron effects at the 60° detection angle in the absence of the target crystal. The only measured difference between the LINAC conditions is found in the Saturation Peak count rate with the LINAC on, which changes the count rate by a factor of 3. More important, the detector detection of the 6.4 keV X-ray is not degraded when the RF is "on" or when the LINAC is "on." When the detector is gated, the 6.4 keV count rate is dramatically reduced since the detector is only active 70 μ s out of the 250 ms between pulses.

4.2.2. Si (220) in Laue and Asymmetric Laue Geometries.

The experimental setup for this experiment is similar to the first PXR experiment except that the electron beam current was kept about a factor of 10 lower, and the ADC was set to 1024 channels. The *Asymmetric Laue* and *Laue* geometries were used for the same Si crystal. Another crystal was modified such that it was cut to a surface dimension of 1 cm x 1 cm with one edge at the manufacturer's <110> flat. This modified crystal was used in the Laue geometry, and it is subsequently referred as the "modified Laue" crystal.

Bragg Angle	30°
Crystal	Si (220), <i>Asymmetric Laue /Laue</i> D= 50mm, t=500 μ m
Predicted Photon Energy	6.45 keV
Electron Energy	50 MeV
Current	45 nA
Comments	Flat at 45° and 0° to horizontal
LINAC Window	Al Water Cooled
Date	15 May 2002

4.2.2.1. Data Analysis

A qualitative argument is presented regarding crystal alignment. For silicon, the absorption length L_a at 13.2 keV is about 200 μ m, so the 500 μ m-thick silicon crystal is $\sim 2.5 L_a$. Using Figure 25, which compares the geometric factor (f_{geo}) as a function of crystal thickness, the expected intensity ratio of PXR from the *Laue* geometry to PXR from the *Asymmetric Laue* geometry would be on the order of 1.5. The most intense Si (440) peaks from the two geometries occur at different energies, but with comparable

count rates. The next higher order, Si (660) is more intense with the *Asymmetric Laue* geometry. An assessment of the quality of the experimental alignment can be determined with the count rate of the next higher order PXR peak. In this experiment, the photons counted in the Si (660) peak have no possibility of pile-up of the lower order PXR photons and are solely attributable to the Si (660) diffraction plane. As a rule of thumb, detection of these higher-order PXR under such conditions represents a better electron-crystal-detector alignment. In this case, conditions in the *Asymmetric Laue* geometry were better aligned than in the Laue case. In fact, in Figure 62 the forth order PXR, Si (880), peak is visible.

Figure 62- Si (220) in *Asymmetric Laue* geometry with $\theta_B=30^\circ$. Electron beam current is 45 nA.

Figure 63- Comparison of Si (220) in *Asymmetric Laue* and *Laue* geometries with θ_B near 30° . Electron beam current is 45 nA.

For each of the three crystal configurations, spectra was collected near $\theta_B=30^\circ$ by rotating the crystal. The Si (220) PXR is not detectable due to air attenuation. Table 19 shows data for conditions providing the most intense Si (440); the Si (440) energies, Si (440) count rates, and Si (660) count rates are shown. In each case, the Si (660) peak can be identified, but its count rate cannot always be measured without large error. An additional peak is observed in each of the spectra at 22.2 keV, and its energy does not change with crystal rotation. This peak's energy corresponds to the fluorescence from the silver K_α transition. The Si detector has a small ring of silver serving as a collimator at the perimeter of the silicon active area, and the fluorescence is from this silver material.

The surface area of the crystal used in the *Asymmetric Laue* and *Laue* geometries is 19.6 cm^2 . Yet when the modified Laue crystal was cut to 1 cm^2 , its measured PXR yield was just reduced by a factor of two. The fact that PXR was generated with such a small crystal is interesting, and may correlate with the usable electron beam area. The RPI LINAC has an electron beam spot diameter of approximately 1 cm at the output window, and it is expected to be bigger at the crystal location, 11.75" away. Future use of small crystals, comparable to the electron beam spot size, will demand a means to align the crystal with the electron beam during PXR experiments.

Table 19. Summary of most intense Si (440) peak count rates measured from the three crystal configurations.

<i>Crystal</i>	<i>Si (440) Energy</i>	<i>Si (440) Rate</i>	<i>Si (660) Rate</i>
<i>Asymmetric Laue</i>	13.4 keV	1.2 cps	0.7 cps
<i>Laue</i>	13.2 keV	1.4 cps	Not Measurable
<i>Modified Laue</i>	13.2 keV	0.6 cps	Not Measurable

4.2.2.2. Conclusions

The level of system alignment can be assessed by the count rates of higher order PXR peaks. This higher count rates can either represent measurement of the higher order PXR photons or the conditions of pile-up of lower order PXR photons. In any event, this still provides a measure of the quality of the alignment of the electron beam with the crystal and the detector. Additionally, PXR was produced with a small 1-cm² silicon crystal, which demonstrates the feasibility of using small crystals for future PXR experiments.

4.2.3. Si (220) Asymmetric Laue Geometry with $\theta_B=10^\circ$.

The changes in this experiment were to move the detector to 20° off of the electron direction. This change made the Si (220) PXR measurable at the detector location 9' away from the crystal. The Si crystal was held with its flat at 45° above the horizontal (*Asymmetric Laue* geometry). The crystal was polished on one side. Data were taken separately with PXR emission from the polished side and with emission from the unpolished side.

Bragg Angle	10°
Crystal	Si (220), <i>Asymmetric Laue</i> D= 50mm, t=500 µm
Predicted Photon Energy	18.59 keV
Electron Energy	50 MeV
Current	64 nA
Comments	Flat at 45°
LINAC Window	Al Water Cooled
Date	21 May 2002

4.2.3.1. Data Analysis

Multiple PXR spectra from Si(220) are measured in the asymmetric Laue geometry with the wafer flat rotated 45° from the horizontal, and θ_B is near 10° . The most intense peak occurs near the Bragg angle, and the intensities decrease when the crystal is rotated away from the Bragg angle. Figure 64 shows the different spectra superimposed on one plot as a function of energy. The electron incident angles are shown with the spectra.

Figure 64- Multiple spectra measured with PXR emission from the polished surface using Si (220) in *Asymmetric Laue* geometry. Crystal is rotated about θ_B near 10° . Electron beam current is 64 nA.

The data for this experiment suggests that the measured spectra are contaminated with diffracted bremsstrahlung. For PXR emitted from either the polished surface or from the unpolished surface of the crystal, Figures 65-66 show that for the crystal rotations that increase the incident angle, the measured spectra energies are more in agreement with calculated diffracted bremsstrahlung energies than with PXR energies. For crystal rotations that decrease the incident angle, the divergence of the theoretical diffracted bremsstrahlung energy and PXR energy is less severe. Additionally, in this region the photon energies are lower, and this would foster the filtering of the lower

energy component of a spectrum due to air absorption. It is best to make this assessment in the region with increased the incident angle.

Figure 65- Comparison of measured photon energy with calculated PXR energy and diffracted bremsstrahlung energy for the crystal rotated about the Bragg angle. PXR emission is from the polished side of the crystal.

Figure 66- Comparison of measured photon energy with calculated PXR energy and diffracted bremsstrahlung energy for the crystal rotated about the Bragg angle. PXR emission is from the unpolished side of crystal.

Some distinctions are observed between emissions from the different crystal sides. In Table 20, the FWHM of the measured spectrum at the Bragg angle is appreciably wider in the case of photon emission from the unpolished surface. Additionally, the contamination of the PXR spectrum affects the measured width of the rocking curve. Figures 67-68 shows the measured widths of the rocking curves. In Figure 67, the rocking curves for both cases are shown as a function of photon energy, and the curves are fit to a gaussian to assess their FWHM (~ 2.35 times the standard deviations of the gaussian distribution). The FWHM are 3.11 and 3.59 keV for the unpolished and for the polished side emission, respectively. The smaller rocking curve FWHM in the unpolished side emission represents a more rapid detuning of conditions satisfying diffraction. In any event, the rocking curves are wide compared to the unbroadened rocking curve from the PXR theory.

Table 20. Comparison of most intense measured Si (220) peak emitted from either side of the single side polished crystal.

<i>Emission Surface</i>	<i>Si (220) Energy</i>	<i>Count Rate</i>	<i>FWHM</i>
Polished	18.78	15.5 cps	490 ± 20 eV
Unpolished	18.85 keV	21.9 cps	850 ± 30 eV

Figure 67- Comparison of the energy rocking curves for Si (220) emitted from the polished and from the unpolished crystal face. Crystal is rotated about θ_B near 10° . Electron beam current is 64 nA.

In Figure 68, the rocking curve for the unpolished surface emission is compared to calculated values from PXR theory. This is calculated with use of Equation 31 with a fixed detector location and varying incident angles ϕ to match the conditions of crystal rotations. Appendix J shows the details of this calculation. Corrections for electron beam current, air attenuation, and detector efficiency are added. Figure 68 also demonstrates a disagreement between PXR yield and predicted intensity because the measured values are a factor of 87 less than expected. This large error may be attributable to the system alignment and large spectrum contamination with diffracted bremsstrahlung (DBR). The contamination of the PXR spectrum compelled the design and acquisition of the new Be LINAC output window and the low measured yield was another demand for better electron beam alignment with the crystal and detector.

Figure 68- Comparison of measured and calculated rocking curve for Si (220) emitted from the unpolished surface. The un-broadened calculated curve is reduced by a factor of 87.4 as a fitting parameter. Crystal rotated about θ_B near 10° . Electron beam current is 64 nA.

4.2.3.2. Conclusions

These experiments demonstrated distinctions in the energy linewidth from Si(220) depending on whether the PXR was emitted from a polished surface or from a rough

surface. The emission from the polished surface resulted in a smaller measured energy FWHM and a broader rocking curve. The measured PXR yield from Si(220) does not agree with the predicted value, differing by nearly two orders of magnitude.

4.2.4. Si (111) and Ge (111) Bragg Geometry near $\theta_B=10^\circ$.

The changes in this experiment were to use the Bragg geometry for Si (111) and Ge (111) and to employ the Si detector with different amplification. The detector had external amplification of 1.5 from its power supply, and internal amplification of 3.0 from the MCA using the "unipolar" setting. Recall that the typical settings are for external amplification of 2.2. Identification of the PXR peaks was difficult. With Si, crystal rotation away from the Bragg angle quickly eliminated the PXR, and with the Ge the PXR peak was not observed.

Bragg Angle	10°
Crystal	Si (111)/Ge (111), Bragg D= 50mm, t=500 μm
Predicted Photon Energy	11.4 keV/ 10.9 keV
Electron Energy	50 MeV
Current	160 nA
Comments	Internal Amp, X3
LINAC Window	Al Water Cooled
Date	19-20 September 2002

4.2.4.1. Data Analysis

Figure 69- Measured Si (111) spectrum $\theta_B = 10.7^\circ$. Note higher order PXR and absence of forbidden Si (222). Electron beam current is 160 nA.

Figure 70- Measured Ge (111) spectrum $\theta_B=10^\circ$. Note dominant bremsstrahlung continuum. Electron beam current is 320 nA.

4.2.4.2. Conclusions

In the Bragg geometry, the alignment necessary to find the Si (111) reflection was more time consuming than with Si (220) in the *Laue* or *Asymmetric Laue* geometries. Additionally, while in the Laue geometry the crystal could be rotated nearly 1.5° about the Bragg angle and the PXR was still measurable. Rotation of the crystal quickly lost the Si (111) PXR. In Figure 69, the Si (111), (333), and (444) are clearly visible. Si (222) is absent because it is a forbidden reflection in silicon. In both Figures 69 and 70, the bremsstrahlung continuum is visible, beneath the Si PXR and concealing the Ge PXR. These first experiments with the Bragg geometry demonstrated that along with the PXR interaction, there is also unwanted bremsstrahlung produced in the crystal.

4.3 First experiments with the Be window.

4.3.1. Si (220) Laue Geometry

The changes for this experiment are to use the new Be window with the BCM mounted on the drift tube. All subsequent experiments use this configuration. The early beam monitor used a fixed target facing the electron beam and tilted 45° to the ground so that the emitted light could be reflected from a ground mirror to the heavily shielded video camera. Beam monitoring targets included aluminum, stainless steel, and concluded with quartz. The Si crystal is single side polished and data were taken such that the PXR was emitted from the polished side. Data were also taken from the unpolished side for comparison. A ^{133}Ba source was added to assess the detector performance during LINAC operations. Detector gating was available but not used during data collection of spectra shown below. No correction for detector deadtime is done because our model does not include the addition of another radiation source.

Bragg Angle	10°
Crystal	Si (220), Laue D= 50mm, t=500 µm
Predicted Photon Energy	18.6 keV
Electron Energy	60 MeV
Current	200 nA
Comments	¹³³ Ba with detector
LINAC Window	Be
Date	16 January 2003

4.3.1.1. Data Analysis

Table 21. Effects of gating detector during LINAC pulse. Count rates compared with and without gating.

<i>Condition</i>	<i>Si (220)</i> <i>[cps]</i>	<i>Ba 31 keV</i> <i>[cps]</i>	<i>Saturation</i> <i>[cps]</i>	<i>Total</i> <i>[cps]</i>
No Gating	3.1	23.6	309	445
With Gating	2.9	0.4	303	364

Table 22. Comparison of count rates from ¹³³Ba, 31 keV X-ray under various LINAC and detection conditions.

<i>Condition</i>	¹³³ <i>Ba 31 keV Source</i> <i>[cps]</i>
No Linac	26.5 ± 0.8
RF On	24.9 ± 0.7
PXR near θ _B	24.5 ± 1.0
Detector gating (80µs wide)	0.36 ± 0.03

Figure 71- Measured energies and spectra from Si (220) collected by scanning the incident angle ϕ about $\theta_B=10^\circ$. Electron beam current is 200 nA. Legend shows electron incident angles, ϕ , for the corresponding spectra.

Figure 72- Comparison of energy rocking curves from Si (220) near $\theta_B=10^\circ$ for the Al and for the Be windows. Data corrected for air attenuation and detector efficiency and normalized to peak values.

Figure 73- Comparison of measured photon energy with calculated PXR energy and diffracted bremsstrahlung energy for the crystal rotated about the Bragg angle, $\theta_B=10^\circ$.

Table 23. Comparison of Si (220) FWHM at $\theta_B=10^\circ$ with emission from polished and from unpolished surface.

<i>Geometry</i>	<i>Polished FWHM</i> [eV]	<i>Unpolished FWHM</i> [eV]
Laue	470 ± 10	560 ± 20
<i>Asymmetric Laue</i>	550 ± 10	610 ± 20

4.3.1.2. Conclusions

There are several conclusions to make from this experiment. In Table 21, we can examine the timing of photon events by comparing count rates with and without detector gating. We assume that the Ba 133 has a nearly constant decay rate over the 120s count times. Gating the detector 80 μ s every 250 ms, the detector is off 99.7% of the time. This explains the drop in the Ba 31 keV count rate shown in Table 21. Since the PXR is associated only with the LINAC pulse, little change in the rate is expected when the detector is gated. However, the purpose for gating was to eliminate detection of photon

events or unwanted detector response in the time between LINAC pulses. A measure of this effect is to compare the rates in the saturation peak, which are effectively unchanged when the detector is gated. There are changes in the total count rate, but this is likely dominated by the elimination of photons associated with the Ba source, which contributed at least 50 cps to identified peaks in the un-gated spectrum. The detector's measured counts are dominated by the time period of the LINAC pulse, and very little is measured between LINAC pulses. We conclude that gating the detector is not necessary.

In Figure 71, the energy tunability for Si (220) is linear with changes in ϕ and spans a range of usable photon energies from 14-22 keV with the detector fixed at $\Omega=2\theta_B$. Figure 72 affirms the increase in usable PXR energies by comparing the Be windows energy rocking curve with that for data collected earlier with the Al window. The rocking curve for diffracting X-rays is generally very narrow compared to PXR. This is observed when comparing the rocking curve in Figure 72. The DBR contamination associated with the Al water-cooled window is likely the cause of the narrow FWHM for the Al window. In Figure 73, the energies of the measured photons are in better agreement with PXR energies than with diffracted bremsstrahlung leading to the conclusion that there is little contamination from bremsstrahlung in the measured spectra using the Be window. Finally, the issue of PXR emission from polished and unpolished surfaces is addressed again in Table 23. While the differences are not as dramatic as first seen in the early experiments with the Al window, there are appreciable differences in the FWHM in data taken in the *Laue* geometry and in the *Asymmetric Laue* geometry. For future experiments, when there are single-side polished crystals, the polished side is oriented towards the detector.

4.4 Experiments with small crystals.

Several experiments were done with crystal with small surface area. These are either circular crystal with diameter (D) of 1 cm or square crystals with area (A) of 1 cm². While selection of these crystals was primarily driven by cost or availability, the experiments with their use affect the electron beam capture cross section and limit the effective area from which PXR is emitted from the target. This is especially true for the RPI LINAC with electron beam diameter at least 1 cm. The small crystals cannot be held

in the optical holders. Instead, these small crystals are held in the poster board holders, which are then held in the optical holders.

4.4.1. Graphite

The only change to the typical experimental set-up is that the beam monitoring was done with a 2"-diameter quartz in the early OTR beam monitoring configuration with the video camera at ground level, in line with the electron beam.

Bragg Angle	10°
Crystal	HOPG (002), Bragg A=1 cm ² , t=1 mm
Predicted Photon Energy	10.7 keV
Electron Energy	56 MeV
Current	102 nA
Comments	0.4° mosaicity
LINAC Window	Be
Date	23 January 2003

4.4.1.1. Data Analysis

Figure 74- Measured spectrum for HOPG (002) spectrum $\theta_B=10^\circ$. Electron beam current is 102 nA.

Table 24. Variation in range of incident angles for which higher order graphite PXR is observed. $\theta_B = 10^\circ$

	<i>1st Order</i>	<i>2nd Order</i>	<i>3rd Order</i>
ϕ Range	7-15°	8-12°	9-11°

Figure 75- Comparison of energy data with calculated PXR energy and diffracted bremsstrahlung energy for crystal rotated about the Bragg angle. Detector angle Ω is 20.35° from the fit.

Figure 76- Total counts for HOPG (002) corrected for air attenuation, detector deadtime, and detector efficiency.

Figure 77- Three HOPG(002) spectra with increasing angles from Bragg angle, $\theta_B = 10^\circ$.

4.4.1.2. Conclusions

Multiple orders of graphite PXR are observed in the HOPG(002) spectrum. Again, the degree of crystal alignment can be assessed with the count rates in the higher order PXR. In Figure 74, the diffraction family HOPG [002] orders 1-3 are observed, and Table 24 lists the range for crystal rotation about the 10° Bragg angle for which the higher order PXR are observed. The count rates are relatively high. But compared to earlier PXR from silicon, the graphite PXR has broad linewidths that get wider for higher order PXR. For applications needing narrow X-ray energy spread, the graphite linewidth cause problems.

The mosaicity for graphite would make it one of the most susceptible crystals to diffracting incident bremsstrahlung to the detector. Figure 75 makes it clear that the HOPG(002) peak is not contaminated with diffracted bremsstrahlung. The rocking curve in Figure 76 does not have the symmetry previously seen with other crystals. This may also be due to the mosaicity. Figure 77 shows three spectra for HOPG(002): one at the Bragg angle, the other two with 1 degree sequential rotations from the Bragg angle. The spectra off of the Bragg angles show some structure that appears like two overlapping peaks which broadens the measured energy. This is likely due to the mosaic structure of graphite.

4.4.2. Tungsten and Copper Crystals

These small metallic crystals were tested with large Bragg angles in order to minimize the detection of bremsstrahlung. There was no detector gating. The crystals are double-side polished.

Bragg Angle	30°
Crystal	W(222),Cu(111), Bragg D=1 cm, t=1 mm
Predicted Photon Energy	13.6 keV/5.3 keV
Electron Energy	50 MeV
Current	Various
Comments	None
LINAC Window	Be
Date	19 March 2003

4.4.2.1. Data Analysis

Figure 78- Tungsten PXR spectrum showing W(222) and W(444) as well as the more dominant L fluorescence lines, $\theta_B = 30^\circ$. Electron beam current is 200 nA.

Figure 79- Copper PXR spectrum showing Cu(222), Cu(333), Cu(444) as well as more the dominant K fluorescence lines, $\theta_B = 30^\circ$. Electron beam current is 585 nA.

Figure 80- Comparison of copper energy data with calculated PXR and diffracted bremsstrahlung energies for crystal rotated about the Bragg angle. Detector angle Ω is 59.6° from the fit. Note the limited range of energies in the data set.

Table 25. BCM measured electron beam currents and Cu K_{α} deadtime corrected count rates for Cu $\langle 111 \rangle$ experiments at $\theta_B = 30^\circ$.

<i>Beam Current</i>	<i>Cu $K_{\alpha 1}$ CPS</i>	<i>Saturation CPS</i>	<i>Total CPS</i>
166 nA	1.31 ± 0.06	9	31
422 nA	1.45 ± 0.07	22	65
585 nA	3.60 ± 0.10	21	64

4.4.2.2. Conclusions

The florescence lines dominated the spectra for both W and Cu. Additionally, background under the measured peaks is relatively large and the bremsstrahlung continuum is easily observed. Spectra taken about the Bragg angle was not possible for W and limited with Cu. Figure 80 attempts to compare the Cu (222) energy data with predictions of PXR and bremsstrahlung, but the limited range of data makes it impossible to conclude whether or not the spectra is PXR. The tunability was so limited that no rocking curve was measured. These spectra for W and Cu demonstrated their limited use with the RPI LINAC. While these crystals offered the best opportunities to obtain high energy PXR, the detection of PXR is so severely complicated by the crystal's bremsstrahlung and florescence that no further experiments with W and Cu were done at RPI.

The detected florescence should offer information about the electron beam current. A similar technique was used by Fiorito, *et al.* when a Zr foil was added to the backside of the PXR crystal to check detector energy calibration and monitor relative electron beam current [56]. Changes in electron beam current should change the detected florescence proportionally. In Table 25, the Cu $K_{\alpha 1}$ deadtime corrected count rates are listed with increasing electron beam current. There seems little correlation between the count rates at the first two electron beam currents. Qualitatively, the rates when the current was 166 nA and 585 nA show some correlation, but nothing is conclusive because of the anomaly at 422 nA. If there were a high total count rate, then detector deadtime may have explained this observation. One possibility is that the electron beam has jitter that moves it on and off this small crystal or the electron alignment with the crystal is altered with changes in electron beam current.

4.4.3. Lithium Fluoride

Small LiF crystals were polished on both of the [100] sides. Recall that the LiF unit cell is cubic. Its symmetry allow for use of LiF (200) parallel with the surface in a Bragg geometry, and use of LiF (200) perpendicular to the surface in a Laue geometry. These experiments collect LiF (200) data in both geometries. These are the first RPI experiments with LiF.

Bragg Angle	30°
Crystal	LiF(200), Bragg & Laue A=1 cm ² , t=1 mm
Predicted Photon Energy	12.3 keV
Electron Energy	50 MeV
Current	617 nA-1.4 μA
Comments	None
LINAC Window	Be
Date	19/26 March 2003

4.4.3.1. Data Analysis

Figure 81 shows a LiF[200] spectrum near the Bragg condition with $\theta_B=30^\circ$. In this PXR spectrum using the Bragg geometry, the 6th order PXR, LiF(12 0 0), is observed. The LiF(200) with energy at 6.20 keV is severely attenuated by the air pathway from the crystal to the detector leaving LiF(400) as the dominant measured peak. Multiple orders of the PXR are observed, and we first discuss deadtime and photon pile-up events so that some comparison can be made between the measured PXR yields and predicted yields normalized to LiF(400).

Figure 81- LiF (200) 1 mm thick in Bragg geometry with $\theta_B=30^\circ$. Electron beam current is 1.26 μA .

If the deadtime correction is applied to the data shown in Figure 81, each of the peak's count rates are increased by a factor of 2. In this experiment, since the first-order PXR LiF(200) is severely attenuated by air, it is not likely that any counts measured in the peak labeled LiF(400) are associated with pile-up of LiF(200) photons. Additionally, the same is true for photons measured in the LiF(600) peak. So in this PXR spectrum, the observed peaks are primarily associated with their corresponding high-order PXR. Ratios are established for the measured counts in a given peak to the measured counts in the LiF(400) peak. The measured and deadtime corrected ratios are the same. This is not true for the photons measured in the peak labeled LiF(800). Photons measured in this peak can be LiF(800) photons or two coincident (LiF)400 photons. For comparison, ratios of theoretical yields (see Equation 31) are determined using the product of the energy dependent frequency, absorption length, and the square of the electric susceptibility ($\omega L_a \chi^2$) with corrections for air attenuation and detector efficiency. Figure 82 shows a log plot of the corrected measured ratios and the theoretical yield ratios for the first three observed higher order PXR peaks in the spectrum shown in Figure 81. As discussed above, the photons in Peak 2 are dominated by LiF(600) photons since there are no possible pile-up events. For Peak 3, there are possibilities of pile-up events; for

example, two coincident LiF(400) photons can be counted in Peak 3. Figure 82 demonstrates that for the first three measured peaks in the spectrum, their relative production is consistent with theoretical predictions. The correction factors to Peak 1 and Peak 2 are the same since there are no pile-up events, and their relative production are not affected by applying the deadtime correction. However, the correction factor for Peak 3 is larger due to the LiF(400) pile-up events. Figure 82 shows the normalized Peak 3 yield without any correction; it does not agree with theory. But when deadtime and pileup corrections are considered, the corrected normalized Peak 3 yield also agrees with the theoretical normalized yield. Further discussion about Peak 4 and Peak 5 is not done because of their low count rates and their more complicated pile-up scenarios, which we have not yet included in the correction model

Figure 82- Corrected counts in the peaks of the LiF(400) and higher order peak (see Figure 81) normalized to the counts in the first peak. Bragg geometry used with $\theta_B=29.25^\circ$, and electron beam current is $1.26 \mu\text{A}$. The theoretical values are shown for comparison.

When the crystal is rotated slightly from the Bragg condition, the PXR energy changes and the number of observed higher-order PXR peaks decrease with greater crystal rotation. This is observed in Figure 83, which demonstrates the linearity of the higher-order PXR energies and the persistence of the higher-order PXR as the crystal is rotated about the Bragg angle. Similar results are seen in the Laue geometry.

Figure 83- Measurement of LiF[200] higher order PXR energy while rotating the crystal about $\theta_B=29.25^\circ$ in the Bragg geometry. Electron beam current is 617 nA.

With the Al, water-cooled window, the measured spectrum was contaminated with diffracted bremsstrahlung (DBR). Now using the 254 μm Be window, a test to determine the diffracted bremsstrahlung contribution is shown in Figure 84 for the Laue geometry. As with the HOPG with $\theta_B=10^\circ$, the LiF(400) energy data agrees better with the PXR energies than with the DBR energies, but the sensitivity of this test is reduced at larger Bragg angles. In this case with $\theta_B=29.25^\circ$, the differences are not as pronounced as at $\theta_B=10^\circ$. As a routine, this test is performed in all PXR experiments, but there will be no further demonstration of this test in this thesis. The Be window is working as designed.

Figure 84- Comparison of LiF(400) energy data with calculated PXR energy and diffracted bremsstrahlung energy for the crystal rotated about the Bragg angle. Detector angle Ω is 59° from the fit. Crystal in Laue geometry.

Next, data were taken with increasing electron beam current with the expectation that the measured PXR count rates would increase proportionally. The measured count rate begins to saturate when the total count rate approaches about 200 cps. The LINAC repetition rate (400 Hz) constrains the total observed count rate to 400 cps. Figure 85 shows the saturation of the measured net counts from LiF(400) in the Bragg geometry as a function of increasing electron beam current. However, after applying the deadtime correction to the measured count rates, the LiF (400) count rates increase linearly with the electron beam current.

Figure 85- LiF (400) net counts with varying electron beam current. Data compared with deadtime corrected values. Crystal in Bragg geometry with $\theta_B=29.25^\circ$.

For small crystals and an assumed negligible mosaicity, the absolute PXR yield can be estimated using the un-broadened PXR photon distribution. A rocking curve was measured for the LiF(400) and the measured net counts in the peak were corrected for detection deadtime, detector efficiency, and air absorption along the route to the detector. This is plotted in Figure 86 as a function of crystal rotation from the Bragg angle. The PXR rocking curve is determined from Equation 31 with the iterative process explained in Appendix J. The LiF(400) yield is then calculated for the electron beam current and the crystal's electron beam capture. This yield is also plotted in Figure 86. While this un-broadened approximation is expected to be inaccurate at the Bragg angle where it calculates zero intensity, the approximation is in good agreement with the magnitude for the net counts and in the width of the rocking curve.

Figure 86- Comparison of LiF(400) rocking curve with un-broadened theory. Data is corrected for air attenuation, detector efficiency, and detector deadtime. Theory accounts for electron beam current and electron beam capture area. Laue geometry with $\theta_B=30^\circ$ and electron beam current of $1.4 \mu\text{A}$.

The first-order PXR yields are sometimes two orders of magnitude greater than the second-order PXR. To this point, discussion has focused on the second-order LiF PXR, but at smaller Bragg angles the detection and use of the first-order PXR will be possible. Even at similar energies, the LiF(400) yield is not comparable to a first order graphite yield. Yet, the quality of this X-ray is worth comparing to graphite, HOPG (002). In Figure 87, PXR from HOPG(002) with $\theta_B=10^\circ$ is shown with PXR from LiF(400) in Laue geometry with $\theta_B=30^\circ$ with an electron beam current about ten times greater. Even though the mosaic spread is the best commercially available at just 0.4° , the graphite energy linewidth is more than twice that of LiF, which is likely dominated by the resolution of the Si detector.

Figure 87- Comparison of LiF[200] spectra in Bragg and Laue geometries with $\theta_B=30^\circ$ and electron beam current of 1.4 μA .

There are some noticeable differences between the Bragg and Laue spectra. Even after optimizing alignment, the Laue geometry seemed to consistently produce higher yields. Figure 88 shows the two spectra measured one after the other with nearly identical electron beam conditions. The net counts in each peak for the two geometries are compared in Table 26. With these small crystals, the electron beam spot is likely larger than the crystal if its face were normal to the beam. In this case, the crystal is rotated so that it captures even less of the electron beam, and the angle of crystal rotation affects the electron beam capture. The Bragg geometry captures less of the electron beam area, and the last column of Table 26 accounts for this by adjusting the Laue net counts normalized to the Bragg geometry. After this correction, the Laue and Bragg net counts are reasonably the same, except in the higher order PXR, which may be due to better crystal alignment in this Laue case. The differences between the Bragg and Laue geometries are much more pronounced when thicker and larger LiF crystals are used.

Figure 88- Comparison of LiF[200] spectra in Bragg and Laue geometries with $\theta_B=30^\circ$ and electron beam current of $1.4 \mu\text{A}$.

Table 26. Net count counts in each PXR peak for Bragg and Laue geometries with $\theta_B=30^\circ$ and an electron beam current of $1.4 \mu\text{A}$. Laue corrected counts are adjusted for electron beam capture by normalizing the results to the Bragg geometry electron capture.

<i>Bragg Energy</i> <i>[keV]</i>	<i>Bragg</i> <i>[Net Cts]</i>	<i>Laue Energy</i> <i>[keV]</i>	<i>Laue</i> <i>[Net Cts]</i>	<i>Corrected Laue</i> <i>[Net Cts]</i>
6.20	50 ± 7	6.23	88 ± 9	51 ± 7
12.37	4448 ± 67	12.42	7451 ± 86	4301 ± 66
18.6	628 ± 25	18.68	1286 ± 36	743 ± 27
24.88	464 ± 22	24.98	1283 ± 36	741 ± 27
31.11	83 ± 9	31.19	367 ± 19	212 ± 15

4.4.3.2. Conclusions

LiF was used for the first time at RPI to produce PXR. Multiple higher-order PXR was observed up to the 6th order from both Bragg and Laue geometries. The first

order PXR, LiF(200) was heavily attenuated by the air pathway from the crystal to the detector so yields were normalized to the most dominant PXR reflection, LiF(400) and measured yields corrected for deadtime and pile-up were consistent with theoretical predictions. Further characterization of the PXR produced from these relatively small (1 cm x 1 cm) crystal was done to include measurement of the rocking curve, examination of effects of increased electron beam current, and comparison of the Bragg and Laue geometries. The low Z LiF crystal offers PXR production with relatively low photon absorption and the advantage of a more narrow linewidth quality than the mosaic graphite.

4.5 Experiments with Thick LiF Crystals.

4.5.1. Bragg and Laue Geometries

Conducting PXR experiments with these larger LiF crystals offer a number of experimental advantages. Unlike the conditions with the small 1 cm x 1cm LiF crystals, the larger crystal size offered some confidence that all of the measured electron beam current is incident on the crystal because the surface area of the crystal is bigger than the electron beam spot. Neglecting electron scattering and energy deposition, the thicker LiF crystal produces greater PXR yields. Most importantly, the thicker crystal allowed the manufacturer (MTI Corporation) to cut the orientation flat at $\langle 110 \rangle$ so that the LiF(220) could be easily aligned for PXR experiments.

The experiments discussed in this section involve some comparison of LiF in the Bragg geometry, LiF(200), and in the Laue geometry, LiF (220). The higher order of the LiF(200) is expected to produce higher PXR yields than LiF(220). But the size of the crystal and the orientation with the electron beam also affects the production of bremsstrahlung photons, which for this work is considered a source of noise. The last part of this section discussed an experiment that seeks to filter this bremsstrahlung with use of an additional analyzer crystal. The modifications to the experimental set-up are shown when this experiment is discussed.

Bragg Angle	15°
Crystal	LiF(200), Bragg LiF(220), Laue D=50 mm, t=1.5 mm
Predicted Photon Energy	11.9/16.8 keV
Electron Energy	57 MeV
Current	Various
Comments	None
LINAC Window	Be
Dates	20-26 August 2003 20-23 October 2003

4.5.1.1. Data Analysis

It can be shown that except in Bragg geometries with small Bragg angles less than 9°, these large LiF crystals capture all of a properly aligned 2-cm diameter, electron beam. There is no scaling of electron beam current when comparing the Laue and Bragg geometries in these experiments with $\theta_B=15^\circ$. Two spectra taken one after the other with no change in the electron beam current are shown in Figure 89. The smaller d-spacing for the LiF(220) produces a higher PXR energy than with LiF(200), but the lower (hkl) with LiF(200) has a higher electric susceptibility producing a greater photon yield. These characteristics are observed as expected in Figure 89. On the other hand, the low saturation peak count rates in the LiF(220) spectrum was unexpected. The LiF(200) saturation peak is nearly six times greater. There is the possibility that a LiF(800) is counted in the saturation peak of the LiF(200) spectrum, however any PXR photon counted at that energy is either a LiF(800) PXR photon or a pile-up event of two LiF(400) photons or three LiF(200) photons. The PXR yields for the higher order LiF(200) photons are relatively low compared to the LiF(200) yield, and the multiple peaks observed in the LiF(200) spectrum are likely to be pile-up events of LiF(200) photons. These measured count rates drop-off by a factor of about two for each succeeding peak, so the PXR photon rate in the LiF(200) saturation peak can be estimated to be up to 10 cps. The remainder is bremsstrahlung.

Figure 89- Comparison of measured LiF(220) spectra in Bragg geometry (upper panel) and LiF(200) spectra in the Laue geometry (lower panel) with $\theta_B=15^\circ$ and electron beam current of 13 nA.

A monte-carlo simulation was done to determine whether there differences in the bremsstrahlung produced from LiF in the two different geometries. The experiments are simulated with a pencil-beam of 56 MeV electrons incident at the appropriate angle to the crystal face, and the bremsstrahlung flux at a point detector is calculated for each of the geometries. No air is used in the simulation. Air would simulate the bremsstrahlung attenuation along the path from the crystal to the detector location. In earlier simulations, the air served more as a bremsstrahlung source along the entire electron path in the simulation geometry, and consequently provided much larger results. The air attenuation can be easily added outside of the simulation. This is done in detail in Section 4.5.3 when the bremsstrahlung is studied in more detail. Nonetheless, adding the air attenuation only affects the soft X-ray component of the bremsstrahlung spectrum. Bremsstrahlung above 40 keV, at which point the air attenuation has dropped to 10%, is

effectively unchanged. Figure 90 shows the simulated LiF bremsstrahlung spectrum. The total bremsstrahlung produced in the Bragg geometry is about an order of magnitude greater than that produced in the Laue geometry. Note that the magnitude of the Si detector response to the bremsstrahlung differences is slightly less due to the detector efficiency. This is because the electron path in the crystal is greater in the Bragg geometry. This has a lot to do with the crystal width. This condition was not observed with the small LiF crystal because the crystal width was about 10 times the crystal thickness, t . In the case with these large crystals, the width is about 30 times the crystal thickness. In the worst case Bragg geometry scenario (θ_B approaches zero), the electron could traverse the entire thickness of the crystal, 50 mm.

Figure 90- Comparison of calculated bremsstrahlung flux at a detector location for the LiF(220) and LiF(200) geometries. Calculation parameters are 56 MeV electrons with the detector 3 m from the crystal.

The comparison of the spectra in Figure 89 continues by assessing the measured PXR yield and comparing it to theoretical predictions. The count rate in the first order peaks for the LiF(200) and the LiF(220) must be corrected for detector deadtime, detector efficiency, and air transmission. The last two corrections are energy dependent. Table 27 shows the first-order peak energy and the associated necessary corrections. The real measured count rate is the deadtime corrected peak rate divided by the detector efficiency

and the transmission through air. This is effectively the PXR photon rate emitted from the face of the crystal. Error in the deadtime corrected rate is calculated using the expression in Appendix K, which shows the error propagation for corrected rates in the first measured peak, the second measured peak, and total measured count rate.

Table 27. Measured count rates for the first order peaks in the LiF(220) and LiF(200) spectra with corrections for detector deadtime, detector efficiency, and transmission through air.

Crystal Plane	Energy [keV]	Measured Peak Rate [Cps]	Measured Total Rate [Cps]	Deadtime Corrected Peak Rate [Cps]	Detector Efficiency	T through Air	Real Count Rate [cps]
LiF(220) Laue	16.56	57.9	85	74 ± 1	0.59	0.66	187 ± 2
LiF(200) Bragg	11.73	98.9	250	264 ± 4	0.92	0.35	830 ± 11

The measured values from Table 27 can now be compared to the expected PXR count rates. The calculated PXR yield is done by integrating about the solid angle subtended by the 3 mm x 3 mm detector collimator using Equation 45. This does not account for PXR broadening. The electron rate is the net electrons per pulse measured by the BCM times the pulse rate of 400 LINAC pulses per second. The error in the electron rate comes from uncertainty in the BCM measurement, in this case 0.2×10^8 electrons/pulse for BCM measurements of 2.0×10^8 electrons/pulse, 10% error. Table 28 shows the calculation of the expected PXR photons rate and the comparison with the measured rate. The two are in reasonable agreement for both cases, although the measured LiF(220) value does not fall within the error limits of the expected value. This reinforces the technique of using the un-broadened photon distribution for determining the PXR yield to first order.

Table 28. Calculated photon rates for the first order peaks in the LiF(220) and LiF(200) spectra. Calculated values are compared with the measured photon count rates.

Crystal Plane	Calculated Yield [photons/e/9mm ²]	Electron Rate [e/s]	Expected Photon Rate [Photon/s]	Measured Count Rate [cps]
LiF(220) Laue	5.75×10^{-9}	$(8.0 \pm 0.4) \times 10^{10}$	230 ± 23	187 ± 2
LiF(200) Bragg	2.19×10^{-8}	$(8.0 \pm 0.4) \times 10^{10}$	872 ± 88	830 ± 11

The next comparison of the two geometries with these two large crystals is with their rocking curves. The rocking curves for LiF(200) and for LiF(220) were measured near the Bragg angle $\theta_B=15^\circ$ but during two different PXR experiment runs with different electron beam currents. LiF(200) was measured in August 2003, and LiF(220) was measured in October 2003. The count rates were corrected for deadtime, detector efficiency, and air attenuation, then normalized to the largest count rate which occurred at the Bragg angle. In Figure 91, the normalized rocking curves are plotted as a function of the crystal rotation angle from the Bragg angle. For consistency, positive rotation angles increase the PXR energy in both plots. Each of the rocking curves were fit to a gaussian distribution and the FWHM is also shown in Figure 91. The widths of the rocking curves are fairly consistent with each other. By comparison, recall that the un-broadened theoretical PXR distribution is defined with the two lobes separated by $\theta_{ph} \sim \gamma^{-1}$, which is 9 mrad for 56 MeV electrons. As expected, the measured PXR FWHM is approximately twice the PXR characteristic angle.

Figure 91- Normalized LiF(200) and LiF(220) rocking curve measured near the Bragg angle $\theta_B=15^\circ$. The electron beam current was 38 nA for LiF(200) and 24 nA for LiF(220).

There are occasions in the PXR experiments when results are better than usual. Below in Figure 92 is a spectrum of the LiF(200) taken within a couple of days of the spectra shown in Figure 89. In this case, the electron beam current was increased by a factor of three, but the counts in the saturation peak are less. This gives evidence that the saturation peak may have a component associated with electron interactions other than with the crystal. There may be "good" electron alignment that eliminates these other interactions. Assuming again that the measured higher-order peaks are primarily LiF(200) pile-up events, the rates drop by a factor of three for each subsequent peak. More notable is the number of measured photons in the first-order peak compared to those in the saturation peak. The ratio of first-order peak count rate to the saturation peak count rate is about three. This is particularly inspiring for an imaging application because the signal to noise is dramatically reduced from what is typically observed. A ratio of one is more often observed.

Figure 92- Measured LiF(200) spectra in Bragg geometry with exceptional signal to noise ratio of nearly 3 to 1. $\theta_B=15^\circ$ and electron beam current of 38 nA.

Filtering is one means to eliminate the photons in the saturation peak. X-ray energy filtering can be done with an analyzer crystal that selectively diffracts X-ray energies to a specific angle governed by Bragg's Law of Diffraction, Equation 4. At RPI, one experiment was done with an analyzer crystal to intercept PXR produced in the typical experimental set-up and to diffract the PXR to another detector location. In the diffraction of polychromatic X-rays, intensity near the diffraction energy can sometimes drop by three to four orders of magnitude solely because of the narrow width of the X-ray rocking curve. For example, a monochromatic 12 keV X-ray has a calculated LiF(200) rocking curve FWHM of $17.5 \mu\text{rad}$ [39]. By comparison, the measured PXR rocking curve was 20 mrad, more than 1,000 times larger. But for nearly monochromatic X-rays like PXR, the reflection coefficient approaches one at the Bragg angle [21]. This alignment is very difficult, but it was done with two additional degrees of freedom. The analyzer is rotated, and the detector at the second detector location is translated. The modified experimental set-up is shown in Figure 93. The PXR crystal is LiF(200) with Bragg angle $\theta_B=15^\circ$, and the analyzer crystal is also LiF(200) so that the PXR is diffracted 15° from its original path. Laser alignment was used to align the analyzer and

to position the second detector, which is lead-shielded with a slit with height 6 mm and width 5 cm. One detector is actually used, first at detector position #1 to tune the primary PXR, then at detector position #2 to measure the diffracted PXR.

Figure 93- PXR reflection experiment using LiF(200) with $\theta_B=15^\circ$ to produce PXR and LiF(200) to diffract PXR.

The size of the PXR beam can be inferred from the PXR rocking curve. This is discussed in the next section, but size of the beam at detector #1 location is about 4 cm at FWHM intensity. In this delicate alignment process, movement of this relatively large primary PXR beam is done first with the goniometer to place the beam on the analyzer crystal and to detect some signal at detector #2. Without this first step, rotation of the analyzer and translation of detector #2 will be unsuccessful in detecting the reflected PXR. Once a signal is detected, detector #2 is translated to find the peak intensity of the reflected PXR. The analyzer is rotated for optimization of the reflected PXR signal. These steps from goniometer adjustment, to translation stage, to rotation stage are

repeated until no further improvement is achieved. In Figure 94, the best reflected PXR spectrum measured at detector position #2 is plotted with the tuned primary PXR spectrum measured at detector position #1. The reflected PXR has a different energy than the primary PXR, and its intensity represents only a third of the primary PXR. The reflected PXR appears as a slice of the primary PXR peak the amount of which is limited by alignment. It may be possible to reflect 100% of the primary PXR beam, but perhaps translation as well as rotation of the analyzer is necessary to do this. This difficult alignment was still achieved, but with a decrease in the PXR count rate. That would be acceptable had the saturation peak been removed. The saturation peak count rates were reduced by using the analyzer, but the signal to noise ratio got worse. This is likely due to the larger slit collimation for detector #2. With the primary PXR, the measured signal to noise ratio was about two measured photons in the first order peak for every saturation peak photon. In the reflected PXR, the ratio dropped to one. Despite this problem, this experiment demands to be repeated with better measures for beam alignment. Additionally, in the reflected spectrum, second order peaks are measured at 23.7 keV. For the analyzer to reflect a monochromatic PXR, the analyzer should be a different crystal than the primary PXR crystal so that second-order PXR are not reflected.

Figure 94- PXR reflection experiment using LiF(200) with $\theta_B=15^\circ$ to produce PXR and LiF(200) to diffract PXR.

Although it is best to not have the second-order PXR, its detection provides more evidence about the true composition of the photons in the second-order peak. The total count rate in the spectrum is 53.6 cps with 18.5 cps in the first-order peak and 1.3 cps in the second-order peak. The deadtime correction model would predict that there are two LiF(400) photons for every LiF(200) pile-up event in the second-order peak, and 20 LiF(200) photons for every LiF(400) photon.

4.5.1.2. Conclusions

This section began as a comparison between the Bragg and Laue geometries for LiF(200) and LiF(220), respectively. There are some inherent differences such as d-spacing and (hkl), which cause PXR energy and yield differences easily predicted by PXR theory. The notable difference between the two geometries is in bremsstrahlung production. The Bragg geometry causes a longer electron path in the crystal and generates about an order of magnitude more bremsstrahlung than the Laue geometry. The rocking curves for the two geometry are equivalent, measured to be about 20 mrad at FWHM and comparable to two characteristic angles, $2\gamma^{-1}$. An exceptional LiF(200) spectrum was measured at $\theta_B=15^\circ$ with a measured signal to noise ratio of three, indicating that there are conditions that can offer better spectra for imaging.

The successful reflection of a primary PXR beam was accomplished with about 33% intensity loss. This successful reflection came with some defeat since the signal to noise ratio dropped from 2 to 1.

4.5.2. X-ray Imaging

X-ray imaging is done with one side of the imaged object nearly flush against the CCD camera face while X-rays are incident on the opposite side of the imaged object. As with every PXR experiment, there are necessary PXR tuning procedures that includes positioning the electron beam on the center of the crystal and rotating and tilting the crystal to maximize the measured first-order PXR count rate. This procedure must be done with the Si X-ray detector with its typical 3 mm x 3 mm collimation. The measurement of an image of this size is not particularly interesting. However, such imaging was done in the initial PXR imaging experiments, and the results are presented

in this section. For more interesting and more realistic imaging applications, the imaged object should be larger. For the remainder of the imaging experiments, the larger 1.6 cm x 1.6 cm collimator is used to shield the CCD camera, which has an active area of 3 cm x 4 cm.

Bragg Angle	15°
Crystal	LiF(220), Laue D=50 mm, t=1.5 mm
Predicted Photon Energy	16.8 keV
Electron Energy	56 MeV
Current	Up to 6.4 μ A
Comments	Large Collimation for CCD Images
LINAC Window	Be
Dates	20 August 2003 8 October 2003 20-21 October 2003

4.5.2.1. Data Analysis

The first attempt to use PXR for imaging with the CCD camera was done with the small 3 mm x 3 mm collimator. As stated above, this is not a particularly interesting approach to image because of the image size. The experiment was primarily intended as a test of the CCD camera and of the photon requirements to image a dense metallic object like a sewing needle. The tests had positive results with the CCD performing as expected with sufficient PXR photons to observe measurable differences between conditions with and conditions without PXR. Figure 95 shows this first image of the eye of a needle viewed through the circular collimator with a 5-mm diameter at the detector end of the small 3 mm x 3 mm collimator. While these images are not very impressive, they demonstrate an apparent difference between the conditions with the PXR and with the PXR de-tuned. Intensity measurements in the area shielded by the collimator are unchanged between the conditions when PXR is on and when PXR is de-tuned. This provides a CCD grayscale background level for this experimental condition. The measurement of direct photons is done in the center of the needle eye. Subtracting the grayscale background level can make a comparison of the direct photon beam with and without PXR. An AOI is established in the eye of the needle with radius of 10 pixels.

The ratio of the net grayscale in the AOI with PXR to without PXR is 1.35, suggesting the level of signal to noise ratio while making this image.

Figure 95- CCD camera image of the eye of a needle using the small collimation (3mm x 3 mm). PXR produced from LiF(400) with $\theta_B=29^\circ$ (12.7 keV) and electron beam current of 640 nA. The left side image is with PXR de-tuned, and the right side image is with PXR at the Bragg angle.

In Figure 96, the large collimator is used to image the metallic sewing needle and a small spring from a ballpoint pen. In this case, LiF(220) is used at $\theta_B=15^\circ$, and the measured first order energy was 16.8 keV. The image at the left is with the PXR de-tuned, and the image at the right is with PXR. Again, the distinction between the image with and without the PXR is clear. The *Photolite* software that accompanies the Gemstar CCD camera allows for quantitative analysis of X-ray images. A "line profile" provides the individual pixel grayscale values across a line of pixels, and the "manual tag" provides integrated RGB intensity of an area of interest with radius of 1-15 pixels. To compare the two situations, three manual tags and one line profile are identified in Figure 96.

Figure 96- CCD camera image of the eye of a needle and a small spring using the large collimation (1.6 cm x 1.6 cm). PXR produced from LiF(220) (16.8 keV) with $\theta_B=15^\circ$ and electron beam current of 960 nA. The left side image is with PXR de-tuned, and the right side image is PXR at the Bragg angle. Exposure time is 5 s.

In Figure 96, the horizontal line marked with a "D" shows the line profile presented in Figure 97 with the PXR on. The left side of this line starts in an area shielded by the detector collimator and proceeds to the right across a region with direct photons, across the eye of the needle, across another region with direct photons, and across a section of the spring. The different regions are clearly visible Figure 97, which plots the pixel grayscale value across a line of about 140 pixels. The CCD has 12-bit grayscale with maximum value of 4095, and in this measurement the areas of direct photons are saturated at the maximum value. The measured grayscale left of pixel location 20 is typical of all of the areas shielded by the detector collimator. This is verified with measurements of the RGB intensity of an area of interest marked "A" in Figure 97 with a 5-pixel radius with PXR on and with PXR de-tuned. Consistently, this background value is unchanged whether the PXR is on or detuned. The background changes only as a function of exposure time and CCD intensifier settings. The peak near pixel location 11 is also repeated whether or not the PXR is on or detuned, and this represents a cluster of bad pixels. A grayscale gradient is seen at the edge of the lead collimator with intensity increasing to the saturation levels with the measurement of direct photons.

Figure 97- Grayscale measurements across the horizontal line of pixels marked "D" in Figure 96 with the tuned LiF(220) PXR at $\theta_B=15^\circ$.

A comparison of grayscale along the line profile "D" with the PXR and with no PXR is shown in Figure 98. In both cases, the grayscale background is about 650 in the area shielded by the collimator. In the imaged area, the grayscale values are reduced when the PXR is de-tuned, and the difference between the two graphs after a background correction represents the contribution from PXR.

Figure 98- Grayscale measurements across the horizontal line of pixels marked "D" in Figure 96 with the tuned LiF(220) PXR at $\theta_B=15^\circ$ shown with a histogram of the grayscale with the PXR de-tuned.

Measurement of RGB intensity is made for circular areas of interest with radii of 5 pixels for conditions with PXR and with PXR de-tuned. Position A is in the image region shielded by the detector collimator and can be considered the grayscale background; Position B is in the image region shielded by the stem of the sewing needle and can be considered the photon transmission through the needle; Position C is in the image region directly exposed the incident photons. Intensity values at Location A are the same for conditions with and without PXR, and this represents a CCD intensity background level for the exposure time and CCD intensification and gain settings for these two images. This value is consistent for any area of interested in the shielded regions of the image. The grayscale saturation values when measuring the direct photons with PXR make it difficult to compare the condition with PXR de-tuned. The intensity ratio should be measured with un-saturated grayscale values.

X-ray imaging with an X-ray energy of 16.8 keV is not difficult to do with relatively thick and dense metallic objects because of large attenuation. Imaging a less dense material is more challenging. In the discussion that follows, LiF(220) is used to produce images of a biological sample (a small fish), a sample with plastic (an electrical switch case), and a semiconductor sample (a computer chip). After analysis of the PXR

used for this imaging, the PXR images are presented and discussed. Figure 99 shows the LiF(220) measured before the X-ray detector was replaced with the CCD camera and before the electron beam current was increased. In this spectrum, the electron beam current was 21 nA, and the calculated deadtime correction to the first-order peak increases the count rate by a factor of two to 164 cps. For the PXR images, the electron beam is increased up to 6.4 μ A, an increase from the spectrum electron beam current by a factor of 300.

Figure 99- LiF(220) spectrum with $\theta_B=15^\circ$ and electron beam current of 21 nA. This spectrum was taken prior to increasing current for PXR the images shown in Figures 103-108.

The LiF(220) rocking curve was measured the day prior to the imaging experiments. The same experimental set-up was used with an electron beam current of 25 nA. In Figure 100, the measured count rates near a Bragg angle $\theta_B=15^\circ$ are plotted as a function of PXR energy and electron incident angle. The peak intensity was measured at 16.6 keV, corresponding to $\theta_B=15.2^\circ$. The energy FWHM of this rocking curve is 0.95 keV. The rotation angle FWHM is 0.9° or 16 mrad.

Figure 100- LiF(220) rocking curve used to characterize the PXR used for imaging near $\theta_B=15^\circ$.

The measured PXR distribution can be assumed to have a gaussian distribution, with peak intensity at the Bragg angle. Any change, $\Delta\phi$, in the electron incident angle due to the crystal rotation moves the Bragg condition. The most intense PXR location moves to a new angular position from the electron direction by $2\Delta\phi$. This fact can be used to infer information about the size of the PXR beam at the fixed detector location. The crystal rotation displacement from the Bragg angle ($\Delta\phi$) can be transformed to distance (Δx) from the Bragg condition at the center of the detector using the expression $\Delta x = R \tan(2\Delta\phi)$. In Figure 101 the transformation was performed on the data shown in Figure 100, and the FWHM of the size of the LiF(220) PXR beam near $\theta_B=15^\circ$ is estimated to be 2.1 cm. This figure also shows vertical lines representing the size of the large collimator wide, across which the PXR intensity drops to just 93% of its peak value. This suggests that the PXR intensity used for imaging is fairly uniform.

Figure 101- Inferred size of the PXR LiF(220) beam at the detector face. Calculated from the rocking curve shown in Figure 100 near the Bragg angle, $\theta_B=15^\circ$.

Finally, the measured count rates in the first-order peak are corrected for detector deadtime, detector efficiency, and air attenuation and plotted in Figure 102 with the theoretical un-broadened yield calculated using Equation 45. There is reasonable agreement between the calculated peak photon yield and the measured PXR yield at the Bragg angle. Of course, Equation 45 does not eliminate the minima at the Bragg angle, but it is an expedient estimate of the PXR yield. Additionally, regardless of the intensity at the Bragg angle, the tails of this estimated photon yield agrees with the measured data at angles far from the Bragg angle.

Figure 102- LiF(220) measured rocking curve with data corrected for detector deadtime, detector efficiency, and air attenuation for incident angles near $\theta_B=15^\circ$. Predicted photon yield using the unbroadened PXR distribution is shown for comparison.

A micro-switch, a computer chip, and a small fish are imaged using the LiF(220) PXR characterized above. For each object, a figure is shown with a digital photograph of the object with the imaged area highlighted, and to the right of the photograph is the X-ray image recorded with no PXR. In the situation with no PXR the crystal rotated 5° from the Bragg angle leaving only the bremsstrahlung from the crystal to produce the images. This figure is then followed by the X-ray image with the PXR.

Figure 103- At the left is the photograph of the 2.5 cm long electrical micro-switch with the 1.6 cm square image area highlighted. At the right is the X-ray image formed with no PXR. The electron beam current is $6.4 \mu\text{A}$ with 20 s exposure time.

Figure 104- PXR image of the electrical switch using LiF(220) with $\theta_B=15^\circ$ and the electron beam current is $6.4 \mu\text{A}$ with 20 s exposure time.

Figure 105- At the left is the photograph of the 4 cm long computer chip with the 1.6 cm square image area highlighted. At the right is the X-ray image formed with no PXR. The electron beam current is $3.2 \mu\text{A}$ with 25 s exposure time.

Figure 106- PXR image of the computer chip using LiF(220) with $\theta_B=15^\circ$ and the electron beam current $3.2 \mu\text{A}$ with 25 s exposure time.

Figure 107- At the left is the photograph of the 6 cm long fish with the 1.6 cm square image area highlighted. At the right is the X-ray image formed with no PXR. The electron beam current is $2.6 \mu\text{A}$ with 15 s exposure time.

Figure 108- PXR image of the fish using LiF(220) with $\theta_B=15^\circ$ and the electron beam current is $2.6 \mu\text{A}$ with 15 s exposure time.

In subsequent PXR imaging experiments, the sustained exposure for the LiF crystal to electron beam currents in the μA -level resulted in fractures along the $\langle 100 \rangle$ direction. To prevent this, a chromel thermal couple is placed in contact with the LiF crystal. The measurement of the temperature is done every second using a Fluke digital multi-meter (DVM) and Fluke software for data acquisition with a PC. The electron beam is turned-on for intermittent periods during which the crystal temperature rises quickly, and then decays exponentially with time until the electron beam is turned-on again. The temperature profile for the LiF crystal with electron beam current at $6.4 \mu\text{A}$ is shown in Figure 109. A long exposure time of 120 s is highlighted in the graph. During this time, the temperature rises by 10.5°C . The mass of the LiF crystal is approximately 7 g and the $1.56 \times 10^3 \text{ J}/(\text{kg}\cdot^\circ\text{C})$. The predicted 4.4 W exposed for 120 s, would result in a temperature change of 48°C . This is a rough estimate without consideration of airflow in the target room and a blower fan placed about 50 cm away from the crystal. The blower worked effectively in bench-top tests with a silicon crystal heated on a hot plate. In this case, the silicon was heated to 170°C on the hot plate and then cooled to an equilibrium temperature of 48°C in about 3 minutes. This was with the blower approximately 10 cm away from the crystal. Unfortunately, this proximity to the LiF crystal held in the cardboard holder generated unacceptable crystal vibration. For future experiments with high electron beam current, a more rigid crystal holder is needed to effectively use the blower to cool the crystal.

Figure 109- Temperature profile of 1.5 mm thick LiF crystal during an imaging experiment using LiF(220) with $\theta_B = 15^\circ$ and the electron beam current is 6.4 μA .

4.5.2.2. Conclusions

For the first time, X-ray images were produced from PXR. LiF(220) with Bragg angle $\theta_B = 15^\circ$ and energy 16.6 keV is used for the imaging. In this Laue geometry, the entire electron beam is placed on this 5 cm diameter crystal, and this was the first time that electron beam currents of μA levels were incident on a PXR crystal. Imaging with PXR still must contend with the background photons that are observed with the PXR detuned. It is likely that this X-ray background is the bremsstrahlung produced by the PXR crystal. In separate experiments, the temperature of the LiF target crystal was monitored. The temperature rises rapidly when the electron beam is on. Crystal cooling and short exposures are necessary to explore PXR with electron beam currents greater than a few μA .

4.5.3. Assessment of LiF Bremsstrahlung

In the PXR spectra measured with the Si X-ray detector, there is a relatively small bremsstrahlung background in the energy region 1-39 keV and a "saturation peak" at the last energy bin of the MCA in which all measured photons above 39 keV are counted. This analysis of the PXR target crystal bremsstrahlung is intended to better understand the source of the saturation peak photons and to quantify these contributions to signal to noise ratio. The assessment of the LiF bremsstrahlung is done primarily by simulating experimental conditions using Monte-Carlo methods and comparing the results with LiF data. Another technique examines the changes in the saturation peak count rates when known absorbers attenuated the incident photon beam on the detector. This is a continuation of the discussion of the differences in the bremsstrahlung produced from the LiF(200) Bragg geometry and the LiF(220) Laue geometry, shown in Figure 90. In this case, further analysis is done to determine the Si detector response to the LiF(220) bremsstrahlung spectrum. The general steps to the Monte-Carlo methods are listed below.

Table 29. Steps to simulating the LiF(220) bremsstrahlung spectrum at $\theta_B = 15^\circ$ measured by the Si detector.

<i>Step</i>	<i>Determined Quantity</i>
1. Simulate the bremsstrahlung flux, $\Phi'_{BS}(E)$, at a point on the detector face (MCNP F5 Tally).	$\Phi'_{BS}(E)$
2. Attenuate the bremsstrahlung flux, $\Phi_{BS}(E)$, for transmission through 274 cm (x) of air.	$\Phi_{BS}(E) = \Phi'_{BS}(E) \cdot e^{-\mu_{air}x}$
3. Normalize the attenuated bremsstrahlung flux energy bin probabilities, $P_{BS}(E)$, for a new simulation source term.	$P_{BS}(E) = \frac{\Phi_{BS}(E)}{\sum_E \Phi_{BS}(E)}$
4. Simulate the Si detector response, $R''_{Si}(E)$, to the normalized attenuated bremsstrahlung flux source term (MCNP F8 Tally).	$R''_{Si}(E)$
5. Normalize the simulated Si detector response, $R'_{Si}(E)$, to units per electron by multiplying by the bremsstrahlung flux probability.	$R'_{Si}(E) = R''_{Si}(E) \cdot \sum_E \Phi_{BS}(E)$
6. Calculate the absolute Si detector response, $R_{Si}(E)$, to the total bremsstrahlung by multiplying the normalized simulated Si detector response by the number of incident electrons, N_e and a detector area scaling-factor, A_D .	$R_{Si}(E) = R'_{Si}(E) \cdot N_e \cdot A_D$

The results from steps 1 and 2 are shown in Figure 110 with a log-log plot of the bremsstrahlung spectrum as a function of energy. The attenuation from air affects the low energy component of the bremsstrahlung spectrum. Above 40 keV, the simulated bremsstrahlung flux and the air attenuated are effectively equivalent. The air attenuates about 16% of the total bremsstrahlung spectrum.

Figure 110- Simulated bremsstrahlung spectrum at the detector using a 1.5 mm thick LiF(220) in Laue geometry with $\theta_B=15^\circ$. The electron energy is 56 MeV. The air-attenuated spectrum is from losses along the 274 cm air pathway.

The air-attenuated spectrum is used as the input source term to determine the Si detector response to the bremsstrahlung. The simulation result is the response per bremsstrahlung photon, which needs to be normalized to a response per electron. Multiplying the simulation result by the bremsstrahlung photon efficiency per electron does this conversion. Figure 111 shows the simulated detector response per electron using the conversion factor of 1.0×10^{-8} photons per electron per cm^2 . Recall that the saturation peak is typically for energies greater than 40 keV, and in the simulation the Si detector measures about 1 count in the saturation peak for every 10 counts in the remainder of the spectrum (<40 keV). Results in Figure 111 can be used to compare the ratio of any measured energy region of a LiF(220) spectrum to the measured saturation peak for the experimental conditions used in this simulation.

Figure 111- Simulated detector response to bremsstrahlung spectrum from a 1.5 mm thick LiF(220) in Laue geometry with $\theta_B=15^\circ$. Normalization factor from flux calculation is 1.0×10^{-8} photons per electron per cm^2 .

For the LiF(220) spectra shown to this point, the PXR count rates have been relatively high and the spectrum background is not observed because of the scale of the graph. However, when the spectra are examined with more detail, the shape seen in Figure 111 becomes very familiar. The data closely resembles the simulation results. The spectrum shown here for comparison was taken with LiF(220) with the crystal rotated by decreasing the electron incident angle (ϕ) by 2.5° from the Bragg angle, $\theta_B=15^\circ$. This detunes the PXR and minimizes the measured PXR whose energy happens to be at about the peak energy (~ 15 keV) of the detector response to the bremsstrahlung shown in Figure 111. The remaining PXR peak is manually stripped from the spectrum; its location is seen in Figure 112 where the bremsstrahlung is flat for the 400 eV span. The electron current is $24 \text{ nA} \pm 10\%$, and the detector response can be calculated with this electron rate, spectrum count time (120s), a scaling for the collimator area (0.09 cm^2). The spectrum is corrected for deadtime with a scaling factor of 1.65 determined from the measured count rate in the bremsstrahlung peak and the measured total count rate. After all of these corrections, the simulated response was larger than the measured response. In Figure 112, to fit the simulated response to the data an additional

normalization factor of four is used to reduce the simulated response values. In the region with energy less than 7 keV, the simulated response shape does not agree well with the measured response. This is likely due to the incorporation of the air attenuation in the simulation model, Step 2 in Table 29. For these energies, the bremsstrahlung transmission through air is very small, just 10^{-6} for 5 keV photons. Consequently, large uncertainty is expected in the simulation in this energy region, and more attention should be given to energy region above 7 keV where the primary detector response is observed. Although the absolute bremsstrahlung calculation has some systematic error that overestimates the bremsstrahlung, the shapes of the measured and simulated responses agree nicely for energies greater than 7 keV. If we assumed that all of this modeling is correct, then we might infer the total contribution of the LiF bremsstrahlung photon contribution to the counts in the saturation peak. After the factor of 4 scaling, a sum of the simulated counts with energy greater than 39 keV results in a total of 23 LiF bremsstrahlung photons counted in the saturation peak when nearly 20,000 counts are measured in the saturation peak.

Figure 112- Comparison of the measured and simulated Si detector response to the bremsstrahlung spectrum from a 1.5 mm thick LiF(220) in the Laue geometry near $\theta_B=15^\circ$ with the crystal rotated 2.5° to detune the PXR. Simulated response is reduced by a factor of 4 to fit the data.

If the measured spectrum background and counts in the saturation peak originate from the LiF bremsstrahlung, then regardless of the absolute predictions of the bremsstrahlung simulation, ratios of count rates can be used to compare the spectrum data to the simulated data. Consider a region of interest (ROI) 16-25 keV for comparison to the saturation peak counts. This region is chosen where the shape of the data closely resembles the shape of the simulation and the energies for the first-order and second-order PXR peaks are avoided. In Table 30, values for the data are the gross number of counts in the ROI, and values for the simulation are the simulated values before the normalization per electron. The ratios shown are the values for the ROI divided by the values for the saturation peak. There is no correlation between saturation peak counts for the data and for the simulation. In the data, the ratios are all small fractions meaning that counts in the saturation peak are much larger than the measured background in the ROI. Conversely, the simulation results predict that there are very few counts in the saturation peak compared to the simulated background in the ROI. These results are consistent for other examined ROIs.

Table 30. Comparison of measured and simulated LiF bremsstrahlung in the saturation peak with use of ratios of counts in an ROI to counts in the saturation peak.

	<i>Sat Peak</i> <i>E>39 keV</i>	<i>ROI</i> <i>E=16-25 keV</i>	<i>Ratio</i> <i>ROI/Sat</i>
<i>Data</i>	11763	2063	0.18
<i>MCNP</i>	0.0075	0.0470	6.28

The results in Table 30 were a test to see whether the measured counts in the saturation peak are attributable to bremsstrahlung from the LiF crystal. The inconsistency with the bremsstrahlung simulation would indicate that the counts are not dominated by bremsstrahlung from the LiF crystal. In fact, if we assume that the simulation is valid, then scaling the MCNP values to the counts in the ROI can predict the LiF bremsstrahlung contribution to the saturation peak. The total measured counts are 2063 for which the simulation would predict a contribution of 328 counts in the saturation peak, or just 2.7 cps. The measured count rate in the saturation peak was 12.6 cps. Consequently, the counts measured in the saturation peak are not likely to be LiF bremsstrahlung with energy greater than 40 keV.

Two questions arise from this finding. Do the photons counted in the saturation peak have energy greater than 40 keV, and what is the source of the photons counted in the saturation peak? To examine the first question, a 1.6 mm-thick aluminum absorber is placed at the entrance to the small 3 mm x 3 mm collimator, and a transmission measurement is made under similar conditions used for the simulation and data collection discussed above. In this case, the crystal is silicon, Si(220), and the Bragg angle is changed from 15° to 10.5° . Since this is a Laue geometry with a relatively small Bragg angle, the crystal face is nearly normal to the electron beam in both cases. Figure 113 shows the spectrum of Si(220) and the same Si(220) spectrum attenuated by 1.6 mm thick aluminum sample at the beam entrance to the collimator. The attenuation observed with the aluminum absorber provides qualitative information about the energy composition of the photons in the peaks. Measured net count rates are shown in the graph, and Table 31 shows the analysis of these measured rates.

Figure 113- Incident and attenuated PXR spectra from Si(220) with $\theta_B = 10.5^\circ$ and an electron beam current of 36 nA. Aluminum attenuator has thickness of 1.6 mm.

Table 31 presents the measured, deadtime corrected, and predicted transmission values for the two PXR peaks, the saturation peak, and the total counts. At Peak 1, the measured transmission is greater than the predicted transmission value, which is easily explained by

more uncounted first-order photons due to detector deadtime and pile-up when the Al absorber is removed. There are less first-order pile-up photons when the absorber is added. However, a deadtime correction to the first-order count rates would predict a transmission of 0.137, which reasonably agrees with the predicted value at 17.7 keV. At Peak 2, the much smaller measured transmission indicates that the majority of photons in the second-order peak are first-order photons. For the saturation peak, the theoretical transmission is calculated for 38.9 keV, and this would under estimate the theoretical transmission because the photon energies can range from 38.9 keV to 56 MeV. Surprisingly, the measured transmission of the saturation peak is actually lower than the predicted transmission for 38.9 keV photons. This striking result indicates that the energy of photons counted in the saturation peak are lower than originally thought. Some of the counts in the saturation peak attenuated by the aluminum absorber are likely pile-up events for lower energy photons.

Table 31. Comparison of theoretical and calculated transmission coefficients from measured counts in the peaks of the Si(220) spectrum shown in Figure 113. The calculated T includes corrections for detector deadtime and pile-up.

<i>Energy [keV]</i>	<i>Measured T</i>	<i>Calculated T</i>	<i>Predicted T</i>
17.7, Peak 1	0.224	0.137	0.123
35.3, Peak 2	0.131	0.396	0.723
38.9, Sat Peak	0.493	0.302	0.772
Total	0.378	0.302	NA

The source of the counts in the saturation peak may still be associated with bremsstrahlung from the crystal. While this cannot be ruled out, another obvious source of events measured in the saturation peak comes from other electron interactions along the LINAC. There are parts of the LINAC that are habitually activated during normal operations, refer to Figure 35. These include the bending magnet M2, the focusing magnets Q1 and Q2, a slightly misaligned section between M2 and Q1, and the aluminum output window when used. Additionally, we have observed some activation of material near the Be window and goniometer when conducting sustained PXR experiments with μA -level currents. One such observation was done during an imaging experiment, where

thermo-luminescent dosimeters were placed at positions around the BCM, Be window, and detector shielding. A photo of the BCM and its lead shielding, Figure 41, is shown again to demonstrate the TLD placement around the BCM.

Figure 41 - TLD Positions for dose measurements summarized in Table 32.

Table 32 shows the measured dose from approximately 1 hour of LINAC operations with electron beam currents up to 1 μA . Locations near the BCM are shown in the picture above. The other locations are described in the table. The area surrounding the BCM showed some activation as measured by the LINAC hand-held survey meter, but this measurement was not recorded. The radiation at location 1 demonstrates the radiation field emitted along the path of the electron. This is outside measured on the 2" diameter drift tube. The difference between the dose measured at location 1 and 2 indicates that the 2" thickness of lead shielding absorbs some fraction of the incident radiation. But the difference between the dose measured at location 2 and 3 indicates that the BCM is also receiving some dose. The dose continues to decline at the other measured locations further from the BCM. Even at the window, the measured dose is just a quarter of that incident at the BCM suggesting that in this experiment the dominant radiation sources are further upstream in the LINAC. This only qualitatively suggests other sources of noise in the LINAC target room. A further characterization is needed to fully understand what is measured as background to the PXR spectra.

Table 32. Location of thermo-luminescent dosimeters and the measured dose for approximately one hour of LINAC exposure with electron beam current up to 1 μA .

<i>Location #</i>	<i>Description</i>	<i>Dose</i>
1	Before 1st lead of BCM, at top of drift pipe	29,900 Rad
2	After 1st lead of BCM, at top of drift pipe	16,500 Rad
3	Before 2nd lead of BCM, at top of drift pipe	8,900 Rad
4	Bottom of Be window, on flange	4,800 Rad
5	Beam side edge of Pb shielding Be window from detector line of sight	884 Rad
6	Bottom of PXR Pb collimator entrance	9.3 Rad
7	Linac side of Pb detector shielding near rear.	3.3 Rad

4.6. Experiments to Measure the PXR Energy Linewidth.

In most cases, the PXR energy linewidth (FWHM) is smaller than the resolution of the Amptek Si detector. A technique to measure such a narrow energy linewidth uses the transmission of PXR through an absorber at energies around an absorption edge. The calculated transmission can be convoluted with a gaussian photon energy distribution with standard deviation, σ . The fit of the data to the gaussian broadened transmission provides the PXR energy standard deviation, which can be used to determine the PXR FWHM [11]. The FWHM is 2.35σ . The equation for the gaussian broadened transmission, T , is shown below with E_0 the mean PXR energy, σ the energy distribution standard deviation, and E the integration variable, which is integrated about 4σ about E_0 .

$$T(E_0) = \int_{E_0-4\sigma}^{E_0+4\sigma} \frac{1}{\sqrt{(2\pi)\sigma}} e^{-\frac{(E_0-E)^2}{2\sigma^2}} \cdot e^{-\mu(E)x} \cdot dE \quad (64)$$

The criterion for the determination of the energy distribution standard deviation (σ) is the minimization of the Chi Squared χ^2 parameter defined below. For each measured photon energy E_i , there is a measured transmission $(T_{data})_i$ with uncertainty $(\sigma_T)_i$ and a calculated gaussian broadened transmission $T(E_i)$.

$$\chi(\sigma)^2 = \sum_i \left[\frac{T_{Data_i} - T(E_i)}{\sigma_{Data_i}} \right]^2 \quad (65)$$

Numerical methods are used to determine the energy distribution standard deviation (σ) that minimizes the value of $\chi(\sigma)^2$, and the uncertainty in σ is determined from a 10% sensitivity of $\chi(\sigma)^2$ as a function of σ .

The absorber foil is held in a rotation stage, which allows the absorber to be placed in the PXR beam at the collimator entrance and then removed. Measurements with the foil removed are the incident intensity, I_o , and measurements with the foil covering the collimator are the transmitted intensity, I . The transmission coefficient, T , is the ratio I/I_o . With rotation of the PXR target crystal, multiple transmission measurements are made for different energies (E_o) around the absorber edge energy.

4.6.1. Linewidth of LiF(400)

A rotation stage is placed near the entrance to the 3 mm x 3 mm lead collimator so that a 1-mil ($25.4 \text{ mm} \pm 10\%$) thick silver foil can be rotated to cover the collimator and again be removed from the collimator entrance. The $K_{\alpha 1}$ absorption edge for silver is at 25.37 keV. The objective of this experiment is to use the gaussian convolution technique to determine the energy linewidth for the LiF(400) PXR. This is a second order reflection from the LiF[200] family of planes, and the predicted photon yield emitted from the crystal surface is a factor of 9.6 less than the first order LiF(200). The best measured count rate in the second order peak was 5.0 cps (see spectrum in Figure 118), and in the end this count rate was not sufficient to determine the LiF(400) energy linewidth because of such low transmission when the foil was rotated to the collimator entrance. The experiment, however provided insight about the real photon rates for the LiF(200) photons and added further verification to the deadtime correction model. This is discussed in Section 4.7.

4.6.2. Linewidth of Si(400)

A rotation stage was used to move an absorber in and out of the PXR beam. In this case, a 1-mil ($25.4 \text{ mm} \pm 10\%$) thick copper foil is rotated to cover the collimator and

again removed from the collimator entrance. Measurements with the foil removed are the incident intensity, I_o and measurements with the foil covering the collimator are the transmitted intensity, I . The transmission coefficient, T , is the ratio I/I_o . The $K_{\alpha 1}$ absorption edge for copper is at 8.98 keV. The objective of this experiment is to use the gaussian convolution technique to determine the energy linewidth for the Si(400) PXR. The first-order reflection is used in this experiment, and there is sufficient photon flux to make the measurement. The transmission at the high-energy side of the absorption edge drops to 0.001 with the 1-mil thick copper foil. Consequently, some transmission data is lost at higher energies because the transmission through the foil is lost in the spectrum background. In any event, the shape of the measured transmission still provides the necessary information to fit the data to the gaussian broadened transmission.

Bragg Angle	30.55°
Crystal	Si(400), Bragg D=50 mm, t=500 μ m
Predicted Photon Energy	8.98 keV
Electron Energy	Not Measured
Current	1.2 μ A
Comments	None
LINAC Window	Be
Date	15 May 2003

4.6.2.1. Data Analysis

The photon energy used for the edge is around 8.98 keV, which is attenuated to just 9% after propagating 274 cm through air from the crystal to the detector. This demands the relatively high electron beam current of 1.2 μ A. It should be noted that the detector in this experiment is more than 60° off of the electron beam direction, and this is expected to reduce the detection of the forward dominated bremsstrahlung produced in the crystal. Figure 114 shows a spectrum with the Cu foil rotated out of the PXR beam. Although the count rate on the Si(400) peak is not impressive, the low count rate of 72 cps in the saturation peak is noteworthy for such a high electron beam current. At detector angles closer to the electron beam direction ($\theta_B \sim 10^\circ$), the detector total count rate would approach saturation at electron beam currents of a few hundred nA on the same sized silicon crystal.

Figure 114- Si(400) spectrum measured with the Bragg angle $\theta_B=30.7^\circ$, and the electron beam current is $1.2 \mu\text{A}$.

Because the total count rate in the spectrum in Figure 114 is relatively low, the deadtime correction is also small. Table 33 shows the correction factor for the Si(400) photon rate. The correction factor is about 2. More interesting is the rate of Si(400) pile-up and its contribution to the Si(800) peak. Unlike the case with the silver foil with detection angle around 28° (see Table 35), the photons in the second order Si(800) are predominantly Si(800) PXR rather than two Si(400) coincident photons.

Table 33. Deadtime corrections to the Si(400) measured spectra showing measured and corrected count rates, the rate of two-Si(400) photon pile-up events, and the fraction of pile-up events and Si(800) photons counted in the Si(800) peak.

<i>Si(400) Energy [keV]</i>	<i>Measured Si(400) Rate [CPS]</i>	<i>Corrected Si(400) Rate [CPS]</i>	<i>Si(400)) pile-up Rate in the Si(800) Peak [CPS]</i>	<i>Ratio of pile-up to Si(800))</i>
12.46	13.3	27.0	0.9	0.06

The deadtime correction is applied to the Si(400) count rate, and the transmission is determined from the ratio of the Si(400) corrected counts with the 1-mil copper foil absorber and to the Si(400) corrected counts without the 1-mil copper foil absorber. The data, un-broadened transmission for a 25.4 mm copper foil, and the gaussian broadened transmission fit to the data with a gaussian standard deviation of 57 eV are all shown

together in Figure 115. There are seven data point in the energy region of the Cu k-edge energy. The first four of those data points have an appreciable different slope than the slope of the last three data points. Emphasis in the data fit is placed on the low-energy slope of the broadened transmission edge. The persistence of the transmission at photon energies above the edge energy indicate the gaussian nature of the linewidth, but a fit to the slope of those last three data points would systematically increase the resulting energy linewidth, when the results at these energies are more prone to error due to low count rates in the transmission. Explanation of the two data points far from the predicted transmission values is difficult. The data at the intermediate energy between the suspicious data is in good agreement with the fit using $\sigma=57$ eV. Additionally, this fit also agrees with the calculated energy FWHM using Equation 29. From geometric considerations, the calculated energy FWHM is then 90 ± 10 eV, and the measured FWHM is $134 \text{ eV} \pm 56 \text{ eV}$.

Figure 115- Measurement of the Si(400) energy linewidth by fitting the deadtime corrected transmission data to a calculated transmission convoluted with a gaussian energy distribution with FWHM= $134 \text{ eV} \pm 56 \text{ eV}$. Cu foil is $25.4 \mu\text{m}$ thick.

4.6.2.2. Conclusions

This experiment achieved its goal of measuring the energy linewidth of the Si(400) PXR with Bragg angle near $\theta_B=30.55^\circ$. In this experimental geometry, the

energy standard deviation is determined from the convolution of a gaussian linewidth with transmission through a 25.4- μm thick copper foil. The measured FWHM is 134 eV $\pm$ 56 eV, which is consistent with the theoretical calculation of the FWHM. In early PXR experiments, low PXR energies and high photon attenuation in air made the use of such a large Bragg angle not very promising. However, in this experiment, the large angle detection offered the condition of low saturation peak count rates and inherently smaller energy linewidth than at small angle detection

4.6.3. Linewidth of Si(220)

A rotation stage was used again to move the absorber in and out of the PXR beam. In this case, a 1-mil (25.4 mm $\pm$ 10%) thick zirconium (Zr) foil is rotated to cover the collimator and again removed from the collimator entrance. Measurements with the foil removed are the incident intensity, I_o and measurements with the foil covering the collimator are the transmitted intensity, I . The transmission coefficient, T , is the ratio I/I_o . The $K_{\alpha 1}$ absorption edge for zirconium is at 18.0 keV.

Bragg Angle	10.5°
Crystal	Si(220), Bragg D=50 mm, t=500 μm
Predicted Photon Energy	17.7 keV
Electron Energy	57 MeV
Current	64 nA
Comments	None
LINAC Window	Be
Date	20 April 2004

4.6.3.1. Data Analysis

The crystal angle providing the most intense first-order PXR count rate is considered the Bragg condition where $2\phi=\Omega$. Figure 116 is the Si(220) spectrum at the Bragg condition with $\phi=\theta_B=10.5^\circ$ and energy of 17.73 keV. This is near the Zr $K_{\alpha 1}$ absorption edge energy, and the energy tunability from crystal rotation allows the execution of this experiment. In the design of this experiment, the detector position was actually determined for LiF(200) in the Bragg geometry. The measured energy FWHM was nearly 1 keV at 17.5 keV, greater than the resolution of the Si X-ray detector. The actual linewidth is measured directly by the Si X-ray detector. To continue with the Zr foil transmission to determine the energy linewidth would be pointless. Additionally, this

LiF(200) spectrum had a high measured signal to noise ratio with about four counts in the saturation peak for every LiF(220) PXR count. Consequently, the use of LiF(200) was abandoned for this experiment.

In contrast, the Si(220) spectrum in the Laue geometry has a measured signal to noise ratio with about three counts in the saturation peak for every Si(220) PXR count. The FWHM measured directly with the Si X-ray detector is 520 eV at 17.7 keV. Because this width includes contribution from the detector resolution, ~300 eV at this energy, the actual PXR linewidth is likely less than what is measured by the detector.

Figure 116- Si(220) spectrum with Bragg angle near $\theta_B = 10.5^\circ$ and electron beam current of 64 nA.

The standard deviation of the Si(220) linewidth is determined from fitting the deadtime corrected Si(220) transmission data to the gaussian convoluted theoretical transmission at the Zr $K_{\alpha 1}$ absorption edge. Figure 117 shows the result of the fit using a standard deviation (σ) of 230 ± 50 eV. The standard deviation is determined by Chi Squared minimization, and the uncertainty in the standard deviation is determined by a 10% sensitivity in changes in Chi Squared. The dominant geometric energy broadening term is the electron beam diameter (D_e), which is approximately 1.5 cm-2.0 cm. The predicted energy FWHM from this geometric energy broadening is then 540 ± 90 eV. The fit parameter from Figure 117 results in a FWHM of $540 \text{ eV} \pm 120 \text{ eV}$. The FWHM

measured directly with the Si X-ray detector was $520 \text{ eV} \pm 20 \text{ eV}$. This also reasonably agrees with the linewidth measured with the Zr transmission.

Figure 117- Measurement of the Si(220) energy linewidth by fitting the deadtime corrected transmission data to a calculated transmission convoluted with a gaussian energy distribution with standard deviation of 230 eV. Zr foil is 25.4 μm thick.

As in the other linewidth measurement experiments, the deadtime corrections for the spectrum are compared. Table 34 shows the deadtime correction for the spectrum in Figure 116. The correction factor to the first-order PXR count rate is 2.2, and the photons in the second-order peak are primarily first-order pile-up events. In other words, the deadtime corrected second-order PXR count rate is zero.

Table 34. Deadtime corrections to the Si(400) measured spectra showing measured and corrected count rates, the rate of two-Si(400) photon pile-up events, and the fraction of pile-up events to Si(800) photons counted in the Si(800) peak.

<i>Si(220) Energy [keV]</i>	<i>Measured Si(220)) Rate [CPS]</i>	<i>Corrected Si(220)) Rate [CPS]</i>	<i>Si(220) pile-up Rate in the Si(440) Peak [CPS]</i>	<i>Ratio of pile-up to Si(440))</i>
17.73	74.9	161.9	32.8	All pile-up

4.6.3.2. Conclusions

The Si(220) energy linewidth is measured using transmission through a 25.4 μm thick Zr foil. Using this technique, the measured FWHM is of $470 \text{ eV} \pm 200 \text{ eV}$. According to Equation 29, the energy linewidth decreases with increased Bragg angle because of its dependence on $\cot(\theta_B)$. The linewidth measurement of Si(400) at $\theta_B=30.55^\circ$, served to be more narrow than the detector resolution. But in the case of the Si(220) at $\theta_B=10.5^\circ$ and with the RPI LINAC experimental parameters, the linewidth measurement is greater than the detector resolution, and such a tedious transmission experiments is probably not necessary to characterize the PXR linewidth. Clearly, at larger Bragg angles the PXR linewidth becomes narrower as seen in Figure 18, and the transmission experiment is justified. Equation 29 can help to establish a criteria for using the transmission experiment. Let the threshold for using the transmission experiment be when the calculated energy linewidth is less than or equal to half of the detector resolution at the PXR energy. The detector resolution is 350 eV at 17 keV. Using an arbitrary PXR diffraction plane and energy of 17 keV with the RPI LINAC experimental parameters and a 1.5 cm diameter electron beam, the threshold Bragg angle for needing to use the transmission experiment to measure the energy linewidth would be 32° . With the assumed parameters above, Bragg angles below 32° would not need the transmission experiment to measure the energy linewidth, but Bragg angles above 32° require the transmission experiment to measure the energy linewidth. Of course, this discussion is energy specific, and the threshold Bragg angle will change for other energies.

4.7. Experiments to Validate the Deadtime Correction Model.

4.7.1. First-Order Peak Correction

The data discussed in this section comes from a relatively unsuccessful attempt to measure the energy linewidth of LiF(400) using the Ag $K_{\alpha 1}$ absorption edge, at 25.37 keV. During the experiment, transmission data is also collected for photons measured in the LiF(200) peak. These results provide a validation of the first order peak deadtime correction model. The experimental parameters are listed below.

Bragg Angle	14.2°
Crystal	LiF(400), Bragg D=50 mm, t=1.5 mm
Predicted Photon Energy	25.4 keV
Electron Energy	~56 MeV
Current	850 nA
Comments	1-mil silver attenuator
LINAC Window	Be
Date	13 May 2003

4.7.1.1. Data Analysis

The LiF(200) spectrum is shown in Figure 118. Three peaks associated with LiF(200) can be observed. At the LiF(400) energy, there are just 5.0 cps of which some counts are pile-up events of two LiF(200) PXR and others are true LiF(400) PXR. The electron beam current is about as high as acceptable for use of the deadtime correction model, which begins to lose validity near at total measured count rate of 300 cps. Transmission through the 25.4 μm thick silver foil at the high-energy side of the silver absorption edge is just 0.27. This makes the gaussian convolution technique for energy linewidth impractical because of the long times needed for statistically accurate measurements.

Figure 118- PXR spectrum from LiF(200) with $\theta_B=14.2^\circ$ and an electron beam current of 850 nA.

However, the data from this experiment provides valuable information about first order, LiF(200), pile-up and verifies the methods in the deadtime correction model. If there were no pile-up or detector deadtime, the photon transmission for the LiF(200) can be determined with the measured net counts in the peak at the LiF(200) energy. In Figure 119, the measured T is the ratio of the measured LiF(200) net count with the foil to the measured LiF(200) net count without the foil, and the theoretical transmission is calculated for a 25.4 μm thick silver foil. An anomaly is observed when comparing the measured transmission and the expected transmission. There is about 40% error in the measured values. The systematic error that raised the measured transmission above the expected value can be caused by detector deadtime, missing LiF(200) photons in the measurement of I_o .

Figure 119- Comparison of transmission (T) calculated from measured counts in the LiF(200) peak, the predicted T through a 25.4 μm thick silver foil, and limits on T due to 10 % variation in foil thickness.

To assess the cause of this systematic, the detector deadtime correction is applied to determine the real LiF(200) count rate. See Equations 60-63 for deadtime corrections. Figure 120 shows the resulting measured transmission corrected for detector deadtime

and pile-up. The manufacturer's tolerance on the silver foil thickness is 10% [57] and independent measurements with calipers with a resolution of 0.1-mil verify the tolerance. The expected transmission coefficient is plotted in Figure 120 as a tolerance region for thickness of $25.4 \mu\text{m} + 2.54 \mu\text{m}$ (lower tolerance of T) and $25.4 \mu\text{m} - 2.54 \mu\text{m}$ (higher tolerance of T). The deadtime correction lowered the transmission data, and the results all fall within the transmission tolerance of the silver foil thickness.

Figure 120- Transmission calculated from deadtime corrected LiF(200) counts and the theoretical transmission through the upper and lower thickness tolerance ($\pm 10\%$) for a $25.4 \mu\text{m}$ thick silver foil.

The correction for the real first-order PXR photons also accounts for the coincidence of any number of first-order PXR photons. Two first-order coincident PXR photons are measured as one photon second-order PXR photon. The correction for the real second-order PXR photons allows the partition of the photons measured in the second-order PXR peak into the number from coincident first-order PXR photons and the number from the second-order PXR photons [55]. In Table 35, measured and corrected count rates are displayed for different direct LiF(200) PXR spectra with the silver foil removed from the collimator. The LiF (200) energy is shown with the measured and corrected first-order PXR count rates; the correction factor is as large as a 3. Listed as "LiF(200) PU in (400) Peak," the rate of two coincident first-order PXR photons is

calculated using the correction in Equation 62. This quantity is a pile-up rate, and the number of first-order PXR photons in the second-order peak is twice that value. Finally, in order to assess the magnitude of the pile-up events, the ratio of two first-order photon pile-up events to the second order photon events is shown in the last column. These ratios indicate that in most cases, the dominant photons measured in the second order PXR peak actually have the first order PXR energy. This observation will be discussed further in the context of another attenuation experiment in Section 4.6.3.

Table 35. Deadtime corrections to LiF(200) and LiF(400) measured spectra showing measured and corrected count rates, the rate of two-LiF(200) photon pile-up events in the (400) peak, and the ratio of pile-up events and LiF(400) photons counted in the LiF(400) peak.

<i>LiF(200) Energy</i>	<i>Measured (200) cps</i>	<i>Total cps</i>	<i>Corrected (200) cps</i>	<i>LiF(200) PU in (400) peak</i>	<i>Measured (400) cps</i>	<i>Corrected (400) cps</i>	<i>Ratio PU to (400)</i>
12.46	29.39	265	87.08	9.48	4.59	4.12	2.30
12.49	27.02	264	79.47	7.89	4.51	5.37	1.47
12.51	31.47	269	96.09	11.54	5.01	3.76	3.07
12.59	23.18	245	59.82	4.47	3.36	4.20	1.07
12.60	25.25	259	71.63	6.41	3.8	4.37	1.47
12.63	25.02	263	73.05	6.67	3.59	3.81	1.75
12.68	21.63	255	59.67	4.45	2.22	1.67	2.66
12.75	23.43	250	62.48	4.88	3.36	4.08	1.20
12.84	21.49	253	58.48	4.27	2.68	3.02	1.42

The above discussion considered the pile-up under the condition with no silver attenuator. The attenuation reduces the pile-up. A plot of the corrected pile-up rate is shown in Figure 121 as a function of the total measured count rate. With the 1-mil silver attenuator, the pile-up of two first-order PXR photons is negligible compared to the un-attenuated PXR beam, which grows exponentially with the measured total count rate.

Figure 121- Calculation of LiF(200) pile-up photons as a function of the spectrum total measured count rate. The crystal is rotated about the Bragg angle $\theta_B=14.2^\circ$, and the electron beam current is 850 nA.

4.7.1.2. Conclusions

The deadtime correction for the first-order PXR count rate is validated with this absorption data. This is a crucial finding because any comparison of the measured PXR yield to the predicted yield relies on the results of the correction model. Additionally, the magnitude of the first-order pile-up events in the second-order peak is determined indicating that a large part of the second-order peak is actually first-order photons. These calculations provide a decomposition of the photons in the second-order peak. Subsequent experiments will validate the deadtime correction for the second-order PXR count rate.

4.7.2. Second-Order Peak Correction

4.7.2.1. Data Analysis

There is no absorption edge in Zr near the energy of the second-order peaks, 32-38 keV. Yet, when the measured count rates in those peaks are used to determine the transmission coefficient, the transmission data is not consistent for photons with the

second-order peak energies. Figure 122 shows the expected transmission calculated for the second-order peak energy range and the measured second-order peak transmission. The structure of the transmission data is strongly characteristic of an absorption edge. This verifies the conclusions from Table 34; the photons in the second-order peaks are actually first-order pile-up events.

Figure 122- Comparison of transmission data from measured count rates in the second-order peak and expected transmission for photons with second-order peak energies. Zr foil with 25.4 mm thickness and Si(220) crystal with θ_B near 10.5° .

Figure 122 shows convincing evidence that the second order peak is dominated by the first-order pile-up events. A simple test of this theory would be to apply the second-order deadtime correction to the data; the result should be a consistent with the plot of the theoretical transmission. In this case, the data is corrected and compared to the theory. Unfortunately, the pile-up is so dominant that the corrected second-order PXR count rates are negligibly small, fluctuating with positive and negative values about zero.

Another way to verify the correction model is to adjust the theoretical transmission to the predictions from the model and compare it to the data. The correction model allows the partition of the photons in the second-order peak. The first-order pile-up events are the coincidence of two Si(220) photons counted in the second-order peak. The correction model for the Si(220) pile-up uses the measured count rates in the first-

order peak and the total count rate (see Figure 116). These pile-up rates are used to determine the calculated transmission had the photons been measured at the first-order peak energies. The transmission of the photons measured at the second-order peak energies is shown with the calculated transmission of the pile-up first-order photons in Figure 123. The gaussian-broadened theoretical first-order transmission is also shown in Figure 123. Keep in mind, that the energies in this plot are the measured energies in the second-order peaks, but the actual energies of the photons are half of that corresponding to the first-order peaks.

Figure 123- Demonstration of first-order Si(220) characteristics in the photons measured in the second-order peak. Corrected values are for transmission at first order energies. Absorber is 25.4 μm thick Zr foil.

4.7.2.2. Conclusions

Earlier in the linewidth measurements using the silver foil, the deadtime correction for the first order count rate was validated. The results shown in Figure 122 and Figure 123 also validate the correction for the first order pile-up rate in the second-order peak. In this experiment, the photons in the second-order peak are primarily first-order pile-up events. This is accurately predicted with the deadtime model and the prediction is consistent with measured transmission of the photons in the second-order peak.

4.8. Summary of Results

4.8.1. PXR Energy Linewidth

The existing theory on the experimental effects that broaden the PXR energy is broken into two categories: geometric effects and crystal mosaicity effects. Electron beam divergence is widely accepted as a second order effect, which is negligible compared to the geometric and crystal mosaicity effects. I isolated the geometric effects by measuring the energy linewidth of PXR from a silicon crystal, which has no mosaicity. In principle, this verifies the theory for geometric broadening of the PXR energy linewidth and validates the sum of all of the geometric effects that broaden the PXR energy linewidth. Once this is done, the energy linewidth for mosaic crystals can be measured and compared to calculated values. Use of Equation 30 determines the total PXR energy linewidth. The magnitude of the energy broadening due to 0.4° mosaicity is twice the broadening due to the experimental geometry near the Bragg angle of 10° . Even for the best quality highly oriented pyrolytic graphite (HOPG) with 0.4° mosaicity, the Si detector resolution allows the direct measurement of the PXR energy FWHM. For this comparison with predicted values, the summed contributions from geometric and mosaic broadening effects over-estimate the measured energy linewidth. For example, Equation 30 predicts for graphite with 0.4 mosaicity near $\theta_B=10^\circ$ a measured PXR FWHM of $800 \text{ eV} \pm 100 \text{ eV}$. With the Si X-ray detector, the linewidth was $650 \text{ eV} \pm 20 \text{ eV}$. For graphite with larger mosaicity, the over-estimate is more severe. Instead of use an algebraic sum of the geometric and mosaic contributions to broadening, Equation 30 is modified so that the contributions are added in quadrature. The equation is shown below and used for comparison with measured values for the energy linewidth.

$$\left. \frac{\delta E_{PXR}}{E_{PXR}} \right|_{tot} = \sqrt{\left(\frac{\alpha}{\cot \theta_B} \right)^2 + \left(\frac{\delta \theta_{geo}}{\cot \theta_B} \right)^2} \quad (66)$$

4.8.1.1. Summary of Energy Linewidth Results

Table 36 shows the results from the linewidth measurements from PXR produced from two silicon diffraction planes with no mosaicity and two graphite HOPG (002) targets with mosaicity of 0.4° and 3.5° . The linewidth measurements for the silicon PXR

are done using the technique that convolutes the linewidth with the transmission near an absorption edge. The linewidths of the graphite PXR are measured directly with the Si X-ray detector. Predicted values are determined using Equation 30 with $a=0$ for the silicon PXR and using the modification in Equation 66 for the graphite PXR. In each case, the measured values are consistent with the predicted values although even with the modification to Equation 30, the theory still overestimates the measured values for PXR from mosaic crystals.

Table 36. Measured and predicted energy linewidth for Si(400), Si(220), and HOPG(002) with mosaicity of 0.4° and 3.5° .

<i>Crystal</i>	<i>Bragg Angle/ Energy</i>	<i>Mosaicity</i>	<i>Measurement Technique</i>	<i>Measured ΔE [eV]</i>	<i>Predicted ΔE [eV]</i>
Si (400)	30.6° 9.0 keV	None	Cu K_α Line	134 ± 56	90 ± 10
Si (220)	10.5° 17.7 keV	None	Zr K_α Line	540 ± 120	540 ± 90
HOPG (002)	10.2° 10.4 keV	$*0.4^\circ \pm 0.1^\circ$	Si Detector FWHM	650 ± 20	550 ± 80
HOPG (002)	9.7° 10.9 keV	$*3.5^\circ \pm 1.5^\circ$	Si Detector FWHM	1690 ± 40	3900 ± 1600

* Mosaicity provided by manufacture, SPI.

4.8.1.2. Conclusions about the Energy Linewidth Theory

The geometric energy broadening in this experiment is dominated by the contribution from the electron beam spot size. The detector collimator and crystal thickness have a small contribution to geometric energy broadening when the detector distance is relatively large. For these conditions, the expression in Equation 29 adequately determines the PXR energy linewidth due to geometric factors. On the other hand when a mosaic crystal is used for PXR production, Equation 30 demands some modification because it over estimates the PXR energy linewidth. This is especially true for crystals with large mosaicity, such as 3.5° (61 mrad). For the better quality graphite with 0.4° (7 mrad) mosaicity the modification in Equation 66 reasonably predicts the measured energy linewidth. One might recall that the PXR rocking curves typically have

a width of twice the characteristic angle, γ^{-1} , 9 mrad for 56 MeV electrons. With some conjecture, the validity of Equation 66 may rest on the relationship of the characteristic angle and the mosaicity. In this work, Equation 66 was valid when the mosaicity was approximately equal to or less than the characteristic angle. For greater mosaicity, the more narrow measured energy linewidth may be due to the relatively dense concentration of the PXR photon spatial distribution.

4.8.2. PXR Photon Yield

Two techniques are available to calculate the PXR yield at a detector location. Techniques A uses Equation 45 for estimating the absolute photon yield by integrating the differential un-broadened photon yield about a small detector solid angle at the peak of the PXR intensity. Technique B uses Equation 55 to first broadening the PXR photon distribution due to electron beam divergence and crystal mosaicity effects. Then the absolute photon yield is calculated from this expression integrating the distribution about a small detector solid angle centered at the Bragg angle.

4.8.2.1. Summary of PXR Yield Results

Appendix L shows all of the PXR results since introducing the 10-mil Be window. Technique A is used to calculate the PXR yield and then incremental steps are taken to calculate the broadened PXR yield due to (a) mosaicity and electron scattering in the crystal, (b) electron scattering from the output window, and (c) the electron scattering from the air pathway from the window to the crystal. The standard deviation of the electron beam divergence is calculated using the electron interaction length, X , shown in Table 7.

Table 37. A summary of the measured and predicted PXR yields. Predicted yields were calculated from distribution broadening due to electron multiple scattering in the output window, the air pathway, and the crystal.

<i>Crystal</i>	<i>Measured Yield [photons/e/9mm²]</i>	<i>Uncertainty [photons/e/9mm²]</i>	<i>Predicted [photons/e/9mm²]</i>	<i>Relative Error</i>
C002	1.4E-07	2.E-08	6.6E-08	-1.05
Cu222	2.6E-11	5.E-12	2.0E-11	-0.30
LiF222	2.8E-11	5.E-12	3.8E-10	0.93
LiF400Bragg	4.2E-10	7.E-11	2.1E-10	-1.06
LiF400Laue	1.5E-10	2.E-11	2.0E-10	0.28
Si111	5.8E-10	1.E-10	2.0E-09	0.71
Si220	3.2E-10	6.E-11	2.0E-09	0.84
Si220	5.3E-09	1.E-09	2.8E-09	-0.88
Si400	1.1E-10	2.E-11	1.9E-10	0.42
Si440	4.6E-11	8.E-12	1.9E-10	0.76
Si440	1.5E-11	2.E-12	2.0E-10	0.93
W222	3.9E-11	8.E-12	2.3E-11	-0.69
LiF220	2.3E-09	4.E-10	1.7E-09	-0.42
LiF200	9.8E-10	2.E-10	3.8E-09	0.74
LiF200	1.1E-09	2.E-10	3.8E-09	0.70
LiF220	1.8E-10	3.E-11	6.7E-10	0.73
LiF400	1.7E-10	3.E-11	1.8E-10	0.02
LiF220	3.2E-09	6.E-10	1.6E-09	-0.97
LiF220	1.6E-09	3.E-10	8.3E-10	-0.93
LiF220	9.8E-10	2.E-10	1.1E-09	0.13
LiF220	7.7E-10	1.E-10	1.1E-09	0.31
Si220	7.2E-10	1.E-10	1.1E-09	0.37
Si400	3.3E-10	7.E-11	5.8E-10	0.43
Si220	1.1E-09	2.E-10	2.4E-09	0.54
Si220	2.0E-09	4.E-10	2.4E-09	0.17
Si220	1.8E-09	3.E-10	2.4E-09	0.26

4.8.2.2. Conclusions about the PXR Yield Theory

Technique A for calculating the PXR photon yield is an estimate that does not consider the electron beam divergence nor the mosaicity of the PXR target crystal. Consequently, this technique will over estimate the predicted PXR yield, up to a factor of 5.5 in the case of Si(220). The severity of this over-estimate can be affected by the PXR polarization. Recall that at $\theta_B=45^\circ$, the PXR is entirely polarized perpendicular to the diffraction plane with zero intensity in the diffraction plane. The difference in the intensity at the characteristic angle is most accentuated as θ_B approached 45° . In fact, at $\theta_B=30^\circ$ the peak intensity of the un-broadened LiF(400) PXR distribution perpendicular to the diffraction plane is approximately four times greater than in the diffraction plane.

To include the electron beam divergence and crystal mosaicity as in Technique B more accurately predicts the measured PXR yield [34]. In most cases, when the broadening due to electron beam multiple scattering from the output window, the air pathway, and the crystal, the relative errors between predicted and measured values are consistently less than one. In some cases with the LiF, the agreement is within 2% for LiF(400) and 13% for LiF(220). The application of Potylitsyn's model of broadening the PXR distribution agrees reasonably well with the measured PXR yield.

CHAPTER 5

DISCUSSION AND CONCLUSIONS

5.1. Achievement of Project Goals.

The goals established at the beginning of this work are restated here.

- Produce tunable X-rays with a narrow energy linewidth (FWHM)
- Produce X-rays with intensity sufficient to image objects with an X-ray CCD camera in a reasonable amount of time
- Minimize background photons (noise)

This work has achieved the goals of the project. First order energy tunability spans the energy range from 6.5 keV using LiF(200) with $\theta_B=30^\circ$ to 18 keV with Si(220) with $\theta_B=9^\circ$. From these Bragg angles, the PXR energy is continuously tunable with the rotation of the crystal. The energy linewidth for Si(400) was measured as low as 90 eV at 8.9 keV, and sufficiently narrow to probe the absorption edges of Cu, Ag, and Zr. X-ray images were produced for the first time demonstrating sufficient photon production to image inanimate objects in 10-25 s. These are not practical exposure times for imaging with a human patient, but the full capacity of the RPI LINAC has not yet been exploited. Finally, PXR is effectively free of background photons under the peak. Photons counted in the saturation peak are attributable to the target crystal bremsstrahlung although our calculations suggest that there are other unidentified sources of noise in the LINAC target room.

5.2. Significance of this Work.

The significance of this work rests in its experimental achievement and in its contribution to the development or the validation of PXR theory. On a number of occasions, the results in this work are achieved for the first time. The most notable experimental-first was the production of the PXR images. Other noteworthy first-time achievements include (1) the employment of μ A-level electron beam currents when previous high currents were in the nA-level; (2) the recognition of PXR target crystal bremsstrahlung as a noise problem in imaging; (3) the absolute characterization of the target crystal bremsstrahlung spectrum; (4) the production of Cu and LiF PXR; (5) the

experimental comparison of Bragg and Laue crystal geometries; and (6) a two-crystal PXR experiment in which the primary PXR is diffraction from a second analyzer crystal. The experiment with tungsten is second only to another research group's recently published results in 2003 [5]. The detailed experimental study of LiF resulted in the development of a deadtime correction model useful for application in most pulsed spectroscopy analysis. Because other studies of PXR were at much lower electron beam currents, photon pile-up was not prevalent. There was no need for a theoretical model to account for detector deadtime and photon pile-up. The deadtime correction model allows for the estimate of real photon rates in any of the peaks in the PXR spectrum and the real total count rate. In this work, these corrections were as large as a factor of four. The use of the deadtime correction is necessary in the analysis of most spectra measured during this work, and this model enabled the comparison of measured and predicted PXR yield. Using Potylitsyn's theory for PXR distribution broadening due to electron beam divergence and crystal mosaicity, our work developed an algorithm to estimate all of the experimental conditions that affect the measured PXR yield. Our modeling accurately predicted measured results. This is the first experimental validation of Potylitsyn's theory applied to thick crystals, such as the 1.5 mm thick LiF, and the first reasonable agreement of measured and predicted PXR yield for PXR generated in air.

5.3. Future Work.

The experimental achievements and contribution to PXR theory should not stop here. Two problems persist in the RPI PXR experiments. The first is the level of bremsstrahlung that accompanies the arrival of PXR at the detector or camera location. The second is the heating and expected degradation of the PXR yield when the electron beam current is increased. The two problems are related by photon yield.

5.3.1. Addressing Target Crystal Bremsstrahlung.

The magnitude of the target crystal bremsstrahlung production is dependent on the crystal atomic number (Z), the detection angle (Ω), and the electron energy (E_e). An early observation from this work was that low Z target crystals provide the highest PXR yield because of low photon absorption at energies appropriate for soft tissue imaging

(15-25 keV). The low Z targets also minimize the electron multiple scattering in the crystal and the bremsstrahlung production. In this sense, no change should be made with this criterion for the crystal material selection; graphite and LiF remain at the top of the list. However, size and shape do make a difference. The amount of material in the electron beam must be minimized to minimize the bremsstrahlung for a given detector angle and electron energy. Recall in Figure 25 that f_{geo} saturates at different crystal thickness depending on the diffraction geometry. In the Bragg geometry, the photon yield saturates at a crystal thickness 1/4 the required thickness in the Laue geometry. In this work, crystals with 5-cm diameter diminished this Bragg advantage because the electrons also traversed the width of the crystal, generating much more bremsstrahlung than in the Laue case. The best geometry to minimize the target crystal bremsstrahlung is a Bragg geometry with thickness of one absorption length (L_a) and width comparable to the electron beam spots size. For 15 keV LiF(200), this would be a crystal with thickness 1.6 mm and width 1 cm. A Monte-Carlo simulation was done to assess the impact of this change. The simulation used 56 MeV electrons with a beam spot radius of 1 cm and photon detection 3 m from the crystal at 30° from the electron beam direction. The results are shown in Table 38. This simple and practical modification in the crystal size reduces the total bremsstrahlung spectrum by a factor of 5.3.

Table 38. Comparison of bremsstrahlung reduction achievable by reducing the crystal surface area in the Bragg geometry.

<i>1 cm LiF width [photons/e/cm²]</i>	<i>5 cm LiF width [photons/e/cm²]</i>	<i>Bremsstrahlung Reduction Factor</i>
1.7 x 10 ⁻⁸ ± 5%	9.0 x 10 ⁻⁸ ± 3%	5.3

Another alternative measure to reduce the bremsstrahlung might be with changes in the electron energy. The low energy port of the RPI LINAC can produce 18 MeV electrons. The same Monte-Carlo analysis used for the effects of the crystal size can be done again for the effects of reducing the electron energy to 18 MeV. In this case, the bremsstrahlung at the detector position was increased by a factor of 5, which is due to the broader angular distribution of the bremsstrahlung, $\gamma^{-1}=28$ mrad (1.6°). The other adverse consequence of moving to the low energy port is the broadened distribution of PXR which reduces the LiF(200) yield calculated with Equation with $\theta_B=15^\circ$ by a factor of 9.

Although material activation at 18 MeV becomes negligible, nothing else is gained by moving to the low energy port. As a side note, this discussion regards the bremsstrahlung produced by the crystal. Other sources of photons have not been fully characterized, but the move to the low energy port would eliminate detection of electron interactions along the last seven LINAC sections.

The remaining issue is the detection angle Ω . The bremsstrahlung is reduced the farther away the detector is from the electron beam direction. However, the increase in Ω also decreases the PXR energy and the photon yield. For 20 keV PXR, the detection angles ($2\theta_B$) for HOPG(002), LiF(200), and LiF(220) are 10.6° , 17.7° , and 25.1° , respectively. These are relatively small angles for direct PXR detection. Not only is there the risk of detection of scattered 56 MeV electrons, the bremsstrahlung spectrum is greatest in the forward direction. Increasing Ω is not an option. An alternative means to overcome this complication is to place an analyzer crystal down range of the PXR crystal. The analyzer crystal plane must have different d-spacing than the PXR crystal to prevent diffraction of the higher-order PXR. The analyzer reflectivity is high limited only by the PXR beam size on the analyzer crystal, the PXR energy linewidth, and the rocking curve of the analyzer crystal. Earlier, an analyzer crystal was employed with some level of success, see Figure 93. This experiment demands to be revisited because successful results offer tunable, higher energy PXR cleaned of higher-order peaks and bremsstrahlung background.

To summarize, the next steps in the reduction of the bremsstrahlung is to employ the Bragg geometry with a small crystal width and to repeat the PXR reflection experiment. Experiments at the low energy port do not offer any advantage in increasing the signal to noise ratio in PXR spectra.

5.3.2. Addressing Target Crystal Heating.

At high electron beam currents, crystal heating without some intervention will degrade the PXR yield and may damage the PXR crystal. On two occasions, the 1.5-mm thick LiF crystals have suffered a fracture after several minutes of exposure to μA -level electron beam currents. In Figure 109, the temperature of a 1.5-mm thick LiF crystal in the Laue geometry with $\theta_B=15^\circ$ is monitored while exposed to the electron beam current

of $6.4\ \mu\text{A}$. Rapid increases in the crystal temperature are observed with a rate of 0.09°C every second. This heating problem is the greatest challenge to sustained PXR operations. Crystal cooling is necessary. The attempt to cool using a blower fan was disrupted by the mechanical instability of the crystal holder. This cardboard holder must be replaced with a more rigid plastic holder or some other design that minimizes holder material in the electron beam. There are other designs for crystals that complement the cooling, such as large single crystals that have fins or circulating coolant. This is a common practice to dissipate heat in the monochromators used at synchrotron facilities. Figure 124 shows the design of two monochromators: the one on the left has cooling fins, and the one on the right has circulating liquid nitrogen. The design can be applied to PXR with some precaution to insure that the electron beam interacts primarily with the target crystal. A smaller electron beam will make precision electron-crystal interactions more feasible; however, it will increase the local heating and might generate localized crystal damage.

Figure 124- Synchrotron monochromator design with fins at the left and liquid nitrogen coolant at the right.

This heating problem with X-ray machines is mitigated through the use of a rotating anode. This causes electron interactions and heat deposition at constantly changing position on the anode while it rotates. Precision alignment is not necessary with the X-ray machine, and it is much more crucial with PXR. Nonetheless, large

silicon wafers are available with diameter of 6". In a Bragg geometry, these wafers can be rotated much like a rotating anode so that the electron beam is concentrated near the outer radius of the wafer. Rotation of the wafer dissipates the electron energy deposition to the circumference of the wafer. A moving crystal target has never been used for PXR production, but there are current studies using a cyclotron that claim re-circulation of electrons through 3-4 cycles in the production of PXR and transition radiation from thin foils [15]. In a sense, the cyclotron represents an analogy to the rotating wafer, and the alignment challenges should be similar.

5.3.3. PXR Applications.

The energy tunability, polarization, and intensity of PXR make it useful in many medical applications. Admittedly, the PXR photon flux is not comparable to a synchrotron radiation source ($\sim 10^{12}$ photons/s/mrad²/0.1% bw) [6] and it was never the goal of this work to compete with a synchrotron radiation source. To gain some perspective on what might be achievable with the RPI LINAC, theoretical calculations of the predicted yield for idealized experimental conditions are presented. The broadened distribution is used for the calculation using 100 μ A electron beam current, 60 MeV electrons, and no degradation from heating. For these conditions, the total integrated photon yield for 20 keV PXR from graphite (002) is about 10^8 photons/s/mrad²/1% bw without correction for distribution broadening. Three collimation systems are compared: the 3 mm x 3 mm collimator currently used in PXR experiments; a circular aperture with 5-cm radius; and a vertical slit perpendicular to the diffraction plane with width 1 mm and height 10 cm. The small collimation provides directional photons for use in precision X-ray interaction applications. The large circular collimation provides photons for imaging a large object. And the slit produces nearly mono-energetic PXR. In Table 39, the detector is 3 m from the crystal. The graphite is calculated with 0.4° mosaicity and electron beam divergence standard deviation of 17 mrad. The LiF is calculated with no mosaicity and electron beam divergence standard deviation of 22 mrad.

Table 39. Predicted LiF(200) and graphite(002) PXR photon yield for 100 μ A electron beam current. Various collimation schemes are considered for medical applications.

<i>Crystal</i>	<i>Small Collimator</i> <i>3 x 3 mm²</i> <i>[photons/s]</i>	<i>Circular Aperture</i> <i>r=5 cm</i> <i>[photons/s]</i>	<i>Slit Aperture</i> <i>1 mm x 10 cm</i> <i>[photons/s]</i>
LiF(200) 1.5 mm thick	1.6 x 10 ⁶	4.6 x 10 ⁸	1.8 x 10 ⁷
Graphite(002) 1.0 mm thick	1.8 x 10 ⁸	4.9 x 10 ¹⁰	1.9 x 10 ⁸

The photon yields in Table 39 represent collimated usable X-rays in three different application configurations with the crystal 3 m from the collimation. Graphite has the advantage in photon yield. To this point, LiF has been favored over graphite because of graphite's energy linewidth and required small detection angle to the electron beam. The requirement for small angle detection may be worked around with the employment of the new RPI LINAC gun or with the use of an analyzer crystal. Both crystals may offer certain advantages depending on the application. The size of the imaged object and the technique for imaging determine the best crystal. Recall the five PXR applications discussed Chapter 1. To select the optimal X-ray energy for absorption contrast imaging, graphite is best because it provides greater flux and the energy linewidth is not so important. Likewise with a contrast agent, the tunability and flux are more important than a narrow linewidth. For material identification and phased imaging, a monochromatic X-ray beam is a priority. For small samples, the small collimation will define the energy linewidth, and graphite is more favorable because of photon yield. For the same reason, graphite should be used with the slit. For a larger sample with use of the 5 cm collimation, the LiF is more favorable because of its more narrow energy linewidth.

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APPENDIX A

EXAMPLE CALCULATION OF THE ELECTRIC SUSCEPTIBILITY, χ_H .

1. Enter tungsten unit cell dimension, a

$$a := 3.16522 \quad \text{Unit cell dimension [angstrom]}$$

2. Calculate the unit cell volume,

$$V := a^3 \quad \text{Volume in angstroms}^3$$

3. Enter Miller indices, hkl, and calculate the plane's d-spacing, d

$$h := 2 \quad k := 2 \quad l := 2$$

$$d := \left[\left(\frac{h}{a} \right)^2 + \left(\frac{k}{a} \right)^2 + \left(\frac{l}{a} \right)^2 \right]^{-.5} \quad \text{Inter-planar spacing, d in angstroms}$$

4. Calculate the momentum transfer, s.

$$s := \frac{1}{2 \cdot d}$$

5. Use the momentum transfer, s, as an input for the anomalous scattering factors .

Anomalous scattering factors are taken from
http://www-phys.llnl.gov/Research/scattering/fftab_energy_q.html
 using perpendicular polarization and fixed momentum transfer equal to
 the s value calculated above.

6. Save the anomalous scattering factors to an Excel spreadsheet, "Tung", to be imported into this Mathcad worksheet .

$j := 2..1287$	index the elements in the spreadsheet
$E := \text{Tung}^{\langle 0 \rangle}$	Photon energy [keV] in the spreadsheet
$fr := \text{Tung}^{\langle 4 \rangle}$	Real Dispersion Correction
$fi := \text{Tung}^{\langle 5 \rangle}$	Imaginary Dispersion Correction
$fs := \text{Tung}^{\langle 3 \rangle}$	Scattering Factor
$\lambda_j := \frac{1.23925910^{-9}}{E_j}$	Wavelength in meters

7. Calculate the number of atoms per unit cell N , [atoms/cm^3]

$$A := 184 \quad \text{Mass number [g/Mol]}$$

$$\rho := 19.3 \quad \text{Mass density [g/cm^3]}$$

$$N_A := 6.022 \cdot 10^{23} \quad \text{Avagadro's Number [Mol/cm^3]}$$

$$\rho_{\text{atom}} := \frac{\rho \cdot N_A}{A} \quad \text{Atom density [atoms/cm^3]}$$

$$N := \rho_{\text{atom}} \cdot V \cdot 10^{-24} \quad \text{N is number of atoms per unit cell}$$

$$N = 2.003$$

8. Enter A, B, C Cromer-Mann Coefficients from Cornell's Chess web site.

Reference := "http://g-line.chess.cornell.edu/~detlef/x-rays/f0_CromerMann.txt"

$$A := \begin{pmatrix} 29.08180 \\ 15.43 \\ 14.4327 \\ 5.11982 \end{pmatrix} \quad B := \begin{pmatrix} 1.72029 \\ 9.2259 \\ .3217030 \\ 57.056 \end{pmatrix} \quad C := 9.8875$$

$$i := 0..3$$

9. Calculate the atomic scattering, f(s)

$$f(s) := \sum_{i=0}^3 A_i \cdot e^{(-B_i \cdot s^2)} + C$$

$$f(s) = 41.343$$

10. Calculate the real part of χ_o

$$r_0 := 2.8179409210^{-15} \quad \text{in meters}$$

$$f_s := f(s)$$

$$\chi_{0r_j} := -(\lambda_j)^2 \cdot \frac{r_0}{[2 \cdot \pi \cdot (V) \cdot 10^{-30}]} \cdot 2(74 + fr_j)$$

11. Calculate the real part of χ_o dipole contribution to absorption

$$\sigma_{D_j} := 2 \cdot \lambda_j \cdot r_0 \cdot f_{i_j} \quad \text{dipole contribution to absorption}$$

$$\chi_{0i_j} := - \left[\frac{\lambda_j}{2 \cdot \pi \cdot (V) \cdot 10^{-30}} \right] \cdot 2 \cdot \sigma_{D_j}$$

12. Calculate the real part of χ_h

$$r := \begin{pmatrix} 0 & .5 \\ 0 & .5 \\ 0 & .5 \end{pmatrix} \quad \text{Relative location of the two tungsten atoms in the unit cell}$$

$$h := (2 \ 2 \ 2)$$

$$Hr := (h \cdot r)^T \quad \text{Dot product results for the exponential}$$

$$k := 0..1$$

$$B := \sum_k \exp(2 \cdot \pi \cdot i \cdot Hr_k) \quad \text{Calculate exp(ihr)}$$

$$B = 2$$

$$S_{hkl} := \left(\text{Im}(B)^2 + \text{Re}(B)^2 \right)^{.5} \quad \text{Determine the structure factor}$$

$$S_{hkl} = 2$$

$$\chi_{hr_j} := - \left[\frac{(\lambda_j)^2 \cdot r_0}{\pi \cdot (V) \cdot 10^{-30}} \right] \cdot (fs_j + fr_j) \cdot S_{hkl}$$

14. Calculate the imaginary part of χ_h

$$\chi_{hi_j} := - \left[\frac{\lambda_j}{2 \cdot \pi \cdot (V) \cdot 10^{-30}} \right] \cdot \sigma_{D_j} \cdot S_{hkl}$$

15. Calculate magnitude of χ_h

$$\chi_{H_i} := \left[\left(\chi_{hi_i} \right)^2 + \left(\chi_{hr_i} \right)^2 \right]^{.5}$$

APPENDIX B

XOH ON THE WEB, RESOURCE FOR ELECTRIC SUSCEPTIBILITIES, χ_H

Electric susceptibilities for calculating the PXR yield for most crystals used during the RPI PXR experiments come from the *Xoh on the Web*, hosted by Argonne National Laboratory and developed by Sergey Stepanov. The web address to access *Xoh on the Web* is <http://sergey.gmca.aps.anl.gov/>. The input for retrieving the χ_h is the energy of the X-ray, the crystal material, and the diffraction plane. An example input dialogue box is shown below in Figure B.1.

X-ray dynamical diffraction data on the Web - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Search Favorites Media Print Mail

Address http://sergey.gmca.aps.anl.gov/cgi/WWW_form.exe?template=x0h_form.htm Go

Links Customize Links Free Hotmail Windows Free AOL & Unlimited Internet Windows Media

X-rays:

☐ Wavelength (Å): 15

☒ Energy (keV):

☐ Characteristic line: Cu-Kα1 ?

Target:

☒ Crystal: Silicon ?

☐ Other material: ?

☐ Chemical formula: and density (g/cm³):

Reflection:

Miller indices: 2 2 0

Database Options for dispersion corrections dfl, dfl2:

☒ Use X0h data (5-25 keV or 0.5-2.5 Å) -- recommended for Bragg diffraction.

☐ Use Henke data (0.01-30 keV or 0.4-1200 Å) -- recommended for soft x-rays.

☐ Use Brennan-Cowan data (0.03-700 keV or 0.02-400 Å)

☐ Compare results for all of the above sources.

Get X0h! Reset

Figure B.1.- Xoh input for 15 keV, Si(220).

Three variables are used from the output of *Xoh on the Web*: the imaginary part of χ_o (used to determine the X-ray absorption length) and the real and imaginary parts of the Sigma χ_h (used to determine the electric susceptibility). An example output dialogue

box is shown below in Figure B.2. Boxes are added to identify the three output variables used for PXR yield calculations.

Structure :	Silicon
Symmetry :	Cubic
Density (gm/cm ³) :	2.3293
Unit cell constants (Å) :	5.4309 , 5.4309 , 5.4309
Unit cell angles (degr.) :	90.000 , 90.000 , 90.000
Poisson Ratio :	0.2800
Composition: Element -- N_sites (Sites occupation)	Si -- 8 (1.000)
X-ray line :	*none*
Wavelength (Å) :	0.82654
Energy (keV) :	15.
Closest absorption edge (keV) :	1.84 (for element Si)
Database for df_1 , df_2 :	*** X0h (International Tables), 5-25 keV ***
$x_{r0} \cdot x_{i0}$ ($n = l + x_{r0}/2 + i \cdot x_{i0}/2$) :	-0.43168E-05 , 0.29647E-07
δ , η ($n = l - \delta - i \cdot \eta$) :	0.21584E-05 , -0.14823E-07
? Absorption factor (1/cm) and length (um) :	22.537 , 443.72
? Extinction length at TER (Å) :	63.313
? Critical angle for TER (degr., mrad) :	0.11904 , 2.0777 GET THE CURVE !
Reflection :	(2 2 0)
Bragg angle (degr.) :	12.429
Interplanar spacing (Å) :	1.9201
sin(QB) , cos(QB) :	0.21523 , 0.97656
tan(QB) , cotan(QB) :	0.22040 , 4.5372
sin(2*QB) , cos(2*QB) :	0.42038 , 0.90735
Polarization :	Sigma
$ x_{rh} \cdot x_{ih} $:	0.26010E-05 , 0.28446E-07
Phase difference ($x_{rh} - x_{ih}$) :	1.0000 * pi
Relative intensity (x_h / x_0) :	60.255 %
? Symmetric Laue-case extinction length (um) :	31.031
? Symmetric Bragg-case extinction length (um) :	2.1770
? Double-crystal curve FWHM (arcsec., urad) :	3.6099 , 17.502
? Darwin curve FWHM (arcsec., urad) :	2.5526 , 12.375 GET THE CURVE !

Figure B.2.- Xoh output for 15 keV, Si(220).

APPENDIX C

DERIVATION OF THE GEOMETRIC FACTOR, F_{GEO}

This is the derivation of the geometric factor, f_{geo} , which accounts for the PXR loss along the photon escape path out of the PXR target crystal. The derivation assumes that the PXR production is continuous along the un-scattered electron velocity direction ($\vec{v}$) through the crystal and that the PXR emission is at some angle 2ϕ from the electron velocity direction. Consider the general situation shown in Figure B.1. The electron is shown moving towards the top of the figure and traversing a crystal with thickness t with its surface normal $\hat{n}$ rotated an angle α from the electron direction $\vec{v}_e$. At the electron entrance to the crystal, the PXR emission is along the vector $\hat{\Omega}$, and ϕ is the angle made between the electron direction $\vec{v}$ and the crystallographic plane defined by the reciprocal lattice vector $\vec{\tau}$.

Figure C.1.-Drawing of the electron with velocity $\vec{v}$ traversing the PXR target crystal and the emission of PXR along the direction $\hat{\Omega}$.

The aim of this derivation is to determine f_{geo} , the transmission of the PXR through the target crystal as the PXR is generated along the electron path. Let x be the electron position in the crystal, $l(x)$ the photon escape distance out of the crystal, and μ the energy dependent photon linear attenuation coefficient. Then f_{geo} can be defined with the expression below.

$$f_{geo} = \int_{x=0}^{x=\frac{t}{\cos(\alpha)}} e^{-\mu l(x)} dx \quad (C.1.)$$

In Figure C.1., the distance $l(x)$ is greatest at the electron entrance to the crystal ($x=0$) and goes to zero at the electron exit from the crystal ($x=t/\cos(\alpha)$). The relationship between $l(x)$ and x can be seen in the Figure B.2.

Figure C.2.-Drawing showing the dependence of the photon path length $l(x)$ on the electron position in the crystal, x .

$l(x)$ can be defined in terms of the angle β and then substituted back into Equation C.1. for the following expression.

$$f_{geo} = \int_{x=0}^{x=\frac{t}{\cos(\alpha)}} e^{-\mu \cdot \left[\frac{t - x \cdot \cos(\alpha)}{\sin(\beta)} \right]} dx \quad (C.2.)$$

Equation C.2. is now simplified by taking the constants out of the integral.

$$f_{geo} = e^{-\mu \cdot \left[\frac{t}{\sin(\beta)} \right]} \int_{x=0}^{x=\frac{t}{\cos(\alpha)}} e^{\mu \cdot \left[\frac{x \cdot \cos(\alpha)}{\sin(\beta)} \right]} dx \quad (C.3.)$$

Integration of Equation C.3. results in the following equation.

$$f_{geo} = e^{-\mu \cdot \left[\frac{t}{\sin(\beta)} \right]} \left[\frac{\sin(\beta)}{\mu \cdot \cos(\alpha)} \right] \left[e^{\frac{\mu \cdot \cos(\alpha)}{\sin(\beta)} \cdot \frac{t}{\cos(\alpha)}} - 1 \right] \quad (C.4.)$$

Replacing $1/\mu$ with L_a (the photon absorption length) and multiplying the exponential terms in Equation C.4. leaves the following.

$$f_{geo} = L_a \left[\frac{\sin(\beta)}{\cos(\alpha)} \right] \left[1 - e^{-\left[\frac{t}{L_a \cdot \sin(\beta)} \right]} \right] \quad (C.5.)$$

In the case of the Bragg geometry where the diffraction plane is parallel to the crystal surface, the angles α and β are complements such that $\beta=90-\alpha$; the same is true for the Laue geometry where the diffraction plane is perpendicular to the crystal surface. The result is that the first term of Equation B.5. in brackets is one, and the second term for the two cases are simplified in terms of the electron incident angle ϕ . For the Bragg geometry, f_{geo} is shown below.

$$f_{geo} = L_a \left[1 - e^{-\left[\frac{t}{L_a \cdot \sin(\phi)} \right]} \right] \quad (C.6.)$$

For the Laue geometry, f_{geo} is shown below.

$$f_{geo} = L_a \left[1 - e^{-\left[\frac{t}{L_a \cdot \cos(\phi)} \right]} \right] \quad (C.7.)$$

And in the general case for any geometry,

$$f_{geo} = L_a \left| \frac{\hat{n} \cdot \hat{\Omega}}{\hat{n} \cdot \hat{V}} \right| \left(1 - e^{-t / (L_a |\hat{n} \cdot \hat{\Omega}|)} \right) \quad (C.8.)$$

APPENDIX D

EXAMPLE CALCULATION OF THE PXR YIELD ABOUT A GIVEN DETECTOR SOLID ANGLE

1. Using Xoh Database, retrieve set of values for imaginary χ_o and real and imaginary χ_h for some desired set of energies. Save values to an Excel spreadsheet, "LifChi".

$i := 0..17$	18 discrete energies
$EE := \text{LiFChi}^{\langle 0 \rangle}$	Photon energy [keV]
$\chi_{oi} := \text{LiFChi}^{\langle 2 \rangle}$	Imaginary part of χ_o
$\chi_{hr\sigma} := \text{LiFChi}^{\langle 3 \rangle}$	Real part of χ_h
$\chi_{hi\sigma} := \text{LiFChi}^{\langle 4 \rangle}$	Imaginary part of χ_h
$\chi_i := \sqrt{(\chi_{hr\sigma_i})^2 + (\chi_{hi\sigma_i})^2}$	Magnitude of χ_h

2. Define Constants

$h_{\text{bar}} := 6.5810610^{-16}$	Plank's constant divided by 2π [eV]
$c := 2.997 \cdot 10^8$	Speed of light [m/s]
$\omega_i := \frac{EE_i}{h_{\text{bar}}} \cdot 1000$	E in [keV]
$K := \frac{1}{137 \cdot 4 \cdot \pi}$	Fine structure constant divided by 4π

3. Enter the crystal parameters

$w := 1500 \cdot 10^{-6}$	Crystal thickness [m]
$\omega_p := 4.835 \times 10^{16}$	Crystal plasma frequency [rad/s]
$d := \frac{4.0276 \cdot 10^{-10}}{\frac{1}{(8)^2}}$	Crystal interplanar spacing [m]
$\tau := \frac{2 \cdot \pi}{d}$	Magnitude of reciprocal lattice vector
$\theta_{B_i} := \text{asin} \left(\frac{2 \cdot \pi \cdot h_{\text{bar}} \cdot c}{1000 EE_i \cdot 2 \cdot d} \right)$	Bragg angle for given energy [rad]

4. Calculate the characteristic angle, θ_{ph}

$$E_e := 56$$

Enter the electron energy [MeV]

$$\gamma := \frac{E_e}{.511}$$

Lorentz factor

$$\theta_{ph_i} := \left[\frac{1}{\gamma^2} + \left(\frac{\omega_p}{\omega_i} \right)^2 \right]^{.5}$$

Characteristic angle [rad]

5. Incorporate the geometric attenuation factors

$$L_i := \frac{2 \cdot d \cdot \sin(\theta_{B_i})}{2 \cdot \pi \cdot \chi_{oi_i}}$$

Attenuation length [m]

$$F_i := L_i \cdot \left(1 - e^{\frac{-w}{L_i \cdot |\cos(\theta_{B_i})|}} \right)$$

Bragg Geometry:

$$L_i \cdot \left(1 - e^{\frac{-w}{L_i \cdot |\sin(\theta_B)|}} \right)$$

Laue Geometry:

$$L_i \cdot \left(1 - e^{\frac{-w}{L_i \cdot |\cos(\theta_B)|}} \right)$$

Asymmetric Laue:

$$L_i \cdot \frac{\left| \sin \left(45 \cdot \frac{\pi}{180} - \theta_B \right) \right|}{\left| \cos \left(45 \cdot \frac{\pi}{180} - \theta_B \right) \right|} \cdot \left(1 - e^{\frac{-w}{L_i \cdot \left| \sin \left(45 \cdot \frac{\pi}{180} - \theta_B \right) \right|}} \right)$$

6. Calculate the photon yield in the detector solid angle

Φ =Integrate intensity over a 9 mm square, (3x3 collimator), with the detector centered in the diffraction plane and at the character angle perpendicular to the diffraction plane.

$$D := 3$$

Width of collimator [mm]

$$R := 3000$$

Distance from crystal to the detector [mm]

$$\frac{D}{2} \cdot \frac{1}{R} = 5 \times 10^{-4}$$

Angular spread for collimator opening D at distance R

$$\Phi_{B_i} := \int_{\theta_{ph_i} - 0.0005}^{\theta_{ph_i} + 0.0005} \int_{-0.0005}^{0.0005} \frac{(5.809 \times 10^{-4}) \cdot F_i(\chi_i)^2 \cdot \omega_i \cdot \left[\theta_x^2 \cdot (\cos(2 \cdot \theta_{B_i}))^2 + \theta_y^2 \right]}{2.997 \cdot 10^8 (\sin(\theta_{B_i}))^2 \left[\theta_x^2 + \theta_y^2 + (\theta_{ph_i})^2 \right]^2} d\theta_x d\theta_y$$

$$\Phi(E) := \text{linterp}(EE, \Phi_B, E)$$

Linear interpolation for photon yield for any given energy E

$$\Phi(17.42) = 5.7277 \times 10^{-9}$$

Photon yield for any given energy
17.42 keV

$$N_i := \frac{(5.809 \times 10^{-4}) \cdot F_i(\chi_i)^2 \cdot (\omega_i)}{2.997 \cdot 10^8 (\sin(\theta_{B_i}))^2}$$

Total number of photons in PXR
distribution without integrating the shape
terms

$$N(E) := \text{linterp}(EE, N, E)$$

Linear interpolation for total number of
photons for any given energy E

$$N(9.89) = 1.34336 \times 10^{-6}$$

APPENDIX E

EXAMPLE CALCULATION OF ELECTRON BEAM AND CRYSTAL MOSAICITY EFFECTS ON PXR PHOTON DISTRIBUTION

1. Define constants and crystal parameters

$$d := 3.348 \cdot 10^{-10} \quad \text{d-spacing for graphite (002), [m]}$$

$$h_{\text{bar}} := 6.58106 \cdot 10^{-19} \quad \text{[keV-s]}$$

$$\tau := \frac{2 \cdot \pi}{d} \quad \text{reciprocal lattice vector, [1/m]}$$

$$c := 2.997 \cdot 10^8 \quad \text{[m/s]}$$

2. Enter unperturbed incident angle and detector angle

$$\theta_B := 15 \cdot \frac{\pi}{180} \quad \text{Electron incident angle, [rad]}$$

$$\Omega_0 := 2 \cdot \theta_B \quad \text{Detector angle, [rad]}$$

$$E := h_{\text{bar}} \cdot c \cdot \tau \cdot \frac{\sin(\theta_B)}{(1 - \cos(\Omega_0))} \quad \text{PXR Energy, [keV]}$$

$$\gamma := \frac{60}{.511} \quad \text{Enter electron energy, [MeV]}$$

$$\theta_{\text{ph}} := \left(\frac{1}{\gamma} \right) \quad \text{Characteristic Angle, [rad]}$$

3. Define Gaussian distribution functions

$$\sigma_m := 0.4 \cdot \frac{\pi}{180} \quad \text{Standard deviation of Mosaic Spread [rad]}$$

$$\sigma_x := .000001 \quad \text{Standard deviation of electron beam divergence in diffraction plane [rad]}$$

$$\sigma_y := .000001 \quad \text{Standard deviation of electron beam divergence perpendicular to the diffraction plane [rad]}$$

$$F_{\text{eff}}(\zeta_x, \zeta_y) := \exp \left[\frac{-\zeta_x^2}{2 \cdot \sigma_x^2 \cdot \left(1 + 4 \cdot \frac{\sigma_m^2}{\sigma_x^2} \right)} \right] \cdot \exp \left[\frac{-\zeta_y^2}{2 \cdot \sigma_y^2 \cdot \left(1 + 4 \cdot \sin^2(\theta_B) \cdot \frac{\sigma_m^2}{\sigma_y^2} \right)} \right]$$

Broadened Distribution Function

$$\Lambda(\theta_x, \theta_y) := \frac{\left[(\theta_x)^2 \cdot (\cos(2 \cdot \theta_B))^2 + (\theta_y)^2 \right]}{\left[(\theta_x)^2 + (\theta_y)^2 + (\theta_{ph})^2 \right]^2}$$

Un-Broadened Distribution Fuction

4. Determine the Shape of the Broadened distribution function

$$\Lambda_{em}(\theta_x, \theta_y) := \int_{-2 \cdot (\sigma_x^2 + \sigma_m^2)^{.5}}^{2 \cdot (\sigma_x^2 + \sigma_m^2)^{.5}} \int_{-2 \cdot (\sigma_y^2 + 4 \cdot \sin(\theta_B)^2 \cdot \sigma_m^2)^{.5}}^{2 \cdot (\sigma_y^2 + 4 \cdot \sin(\theta_B)^2 \cdot \sigma_m^2)^{.5}} F_{eff}(\zeta_x, \zeta_y) \cdot \Lambda(\theta_x + \zeta_x, \theta_y + \zeta_y) d\zeta_y d\zeta_x$$

Note integration about two standard deviations of this distribution function

Calculate the distribution by making discrete steps in θ_x and θ_y .

$$i := 0..50$$

$$j := 0..50$$

$$\Delta x := 4 \times 10^{-3}$$

$$\Delta y := 4 \times 10^{-3}$$

$$\theta_{x_i} := -0.1 + i \cdot \Delta x$$

$$\theta_{y_j} := -0.1 + j \cdot \Delta y$$

Broadened Distribution

$$N_{i,j} := \Lambda_{em}(\theta_{x_i}, \theta_{y_j})$$

N

Un-Broadened Distribution

$$N1_{i,j} := \Lambda(\theta_{x_i}, \theta_{y_j})$$

N1

5. Normalize the Broadened distribution to the Un-Broadened distribution

$$Tot := \Delta x^2 \cdot \sum_i \sum_j N_{i,j}$$

Calculate the area under the broadened distribution function

$$Norm_{factor} := \frac{\int_{-0.1}^{0.1} \int_{-0.1}^{0.1} \Lambda(\theta_x, \theta_y) d\theta_x d\theta_y}{Tot}$$

The normalization factor is calculated with the ratio of area under the un-broadened distribution function to the area under the broadened distribution function

6. Integrate the Broadened distribution about the detector solid angle

$$S_x := \int_{-0.0005}^{0.0005} \int_{-0.0005}^{0.0005} \Lambda_{em}(Y, X) dX dY$$

Collimation angle 3 mm at 3 m.

$$S_{PXR} := Norm_{factor} \cdot (S_x)$$

Multiply by normalization factor to get the absolute PXR yield per electron

7. Determine the expected PXR yield from the electron beam currents

$$NumPxr := 1.80453 \times 10^{-4}$$

Get this value from all other terms in the differential intensity equation

$$NumPxr \text{ equals } \frac{(5.809 \times 10^{-4}) \cdot F_i(\chi_i)^2 \cdot \omega_i}{2.997 \cdot 10^8 (\sin(\theta_{B_i}))^2}$$

$$P_e := S_{PXR} \cdot NumPxr$$

Photons per electron, P_e

$$Rate_e := \frac{1 \cdot 10^{-6}}{1.6 \cdot 10^{-19}}$$

Electron rate from electron beam current

$$P_s := P_e \cdot Rate_e$$

Photons per second, P_s

$$P_s = 2.40598041 \times 10^6$$

APPENDIX F **EXAMPLE MCNP-4C2 CALCULATION FOR WINDOW EFFECTS** **ON ELECTRONS AND PHOTONS**

```

$Window -- Electrons from 10 mil Be window
1      1  -1.848  1 -2 -3      imp:p=1 imp:e=1  $ Be sheet
2      2  -1.293e-3 2 -4 -3    imp:p=1 imp:e=1  $ air path
3      3  -2.3    4 -5 -3      imp:p=1 imp:e=1  $ SiCrystal
4      0          -99          imp:p=1 imp:e=1  $ air around
          (-1:5:3)
99     0          99          imp:p=0 imp:e=0  $ zero-importance outside world

1      px  0          $Start 10 mil Be
2      px  0.0254      $End 10 mil Be
4      px  30.00762    $Start 500 micron Si
5      px  30.05762    $End 500 micron Si
3      cx  5.0         $5cm diameter of Si Wafer
99     so  32.0

c      electron source
sdef   erg=60.000 pos=0 0 0 sur=1 dir=1 vec=1 0 0 par=3
m1     4000 1          $Be
m2     7000 3 8000 1   $Air
m3     14000 1         $ Si
mode   p e
c
e0     0 99i 61        $Energy of electron [MeV]
fl:e   2              $Surface Current from Be Window
c0     -1.0 0.99 999i 1.0 t $Cosine bins for angles from Be Window
fql    c e            $List tally fl in cos angle bins
c
nps    500000
prdm   2j 1
print
dbcn   156771161

```

APPENDIX G

MCA SETTINGS FOR SI DETECTOR

The Amptek Si detector has its own power supply and amplifier. For all of the PXR experiments, the Amptek amplification was done with the RTD on, and with the amplification set to 2.2. This is "external" amplification for the MCA (multi-channel analyzer). An example of the ApteC Eagle Classic MCA spectrum dialogue window is shown below. Use of the "Setup" dropdown menu provides access to setting the Pre-amplification, Amplification, and ADC (analogue to digital converter).

Figure G.1.- PXR spectrum shown on ApteC MCA window.

Figure G.2.- Preamplifier settings for Aptec MCA.

Figure G.3.- Amplifier settings for Aptec MCA.

ADC Setup for LiF200at76-3.50 [X]

Number of Channels in Spectrum
☐ 256 ☐ 512 ☒ 1024 ☐ 2048 ☐ 4096 ☐ 8192 ☐ 16384

ADC Gain
☐ 256 ☐ 512 ☒ 1024 ☐ 2048 ☐ 4096 ☐ 8192 ☐ 16384

Offset
☒ Internal ☐ External

Internal Channel Offset
☒ 0 ☐ 1024 ☐ 2048 ☐ 3072 ☐ 4096 ☐ 5120 ☐ 6144 ☐ 7168
☐ 512 ☐ 1536 ☐ 2560 ☐ 3584 ☐ 4608 ☐ 5632 ☐ 6656 ☐ 7680

ADC Mode
☒ Normal (Anticoincidence) ☐ Coincidence

Coincidence Input
 Coincidence = ☒ 5V ☐ 0V
☒ Level ☐ Edge Sensitive

Dead Time Input
 Dead = ☒ 0V ☐ 5V

Reject Input
 Reject = ☒ 0V ☐ 5V

Linear Gate Output
 Gate = ☒ 0V ☐ 5V

LLD
 29.72
 2.906 %
 ▲
 ▼

ULD
 1023.00
 100.0 %
 ▲
 ▼

ZERO
 0.0062
 0.001 %
 ▲
 ▼

Pulses Above ULD
☐ Ignore ☒ Place In Last Channel

External Offset Input
 Offset = ☒ 0V ☐ 5V

Defaults Recall User Defaults Save User Defaults OK Cancel

Figure G.4.- ADC settings for Aptec MCA.

APPENDIX H

LASER ALIGNMENT PROCESS FOR POSITIONING THE DETECTOR AND COLLIMATION

This process begins with the crystal positioned in front of the output window so that when all three of the goniometer angles (Ω , α , β) are set to zero, the crystal face is vertical, parallel to the direction of the electron beam, and centered on the output window. The goniometer table is then fixed in place, and the goniometer reference angles are set. The goal of the laser alignment is to position the detector and collimation to this established reference angle. The detector table is positioned generally at the correct angle and distance from the PXR crystal; the detector table top has only the detector aluminum housing with the alignment laser (see Figures 51-52 in the Thesis).

Laser alignment steps.

#	Action	Goniometer, Ω
1	Rotate the crystal so that its face points to the desired detector location	$2\theta_B - 90^\circ$
2	Rotate and translate the alignment laser/detector box so that the laser reflects off of the center of the crystal and enters back into the laser emission face.	$2\theta_B - 90^\circ$
3	Rotate the crystal so that its thin side faces the incident laser and rotate and translate the alignment laser/detector box so that the laser strikes the narrow edge of the crystal. A symmetric diffraction pattern is seen on the opposite side of the crystal.	$2\theta_B$
4	Repeat step 2, and fix the detector box with stacked lead.	$2\theta_B - 90^\circ$
5	Rotate the crystal so that the laser beam is now reflected into the center of the LINAC output window. Repeat steps 2-4 until this is accomplished.	θ_B
6	Return to step 2 and build the collimation so that the laser passes through the collimation, reflects from the crystal, and returns back into the collimation.	$2\theta_B - 90^\circ$

APPENDIX I

EXAMPLE CALCULATION OF THE REQUIRED DISTANCE FROM THE LINAC WINDOW TO THE PXR CRYSTAL

1. Define experimental parameters.

$R := 274$	Distance from crystal to detector [cm]
$\Omega := 30\text{-deg}$	Detector angle [deg]
$L := 40$	Length of the colimator [cm]
$d := .3$	Width of the Colimator [cm]

2. Define calculation variables.

$Y_0 := R \cdot \sin(\Omega)$	y position of the center of the detector
$X_0 := R \cdot \cos(\Omega)$	x position of the center of the detector Origin at crystal with x in direction of e-beam y perpendicular to e-beam
$\Delta y := \frac{\frac{d}{2}}{\cos(\Omega)}$	Change in y at the edge the collimatorer [cm]
$Y_{\text{new}} := Y_0 - \Delta y$	y position at the edge the collimatorer [cm]
$\beta := \frac{\pi}{2} - \Omega$	Angle looking back from detector to crystal [rad]
$\beta_{\text{Add}} := \text{atan}\left(\frac{d}{L}\right)$	Change in β because of the collimator dimension [rad]
$X_{\text{new}} := Y_{\text{new}} \cdot \tan(\beta + \beta_{\text{Add}})$	New x coordinate of viewable region from edge of collimator [cm]

3. Calculation crystal to window distance.

$X := X_{\text{new}} - X_0$	Required distance from the crystal to the window such that the window is not viewed from the collimated detector [cm]
-----------------------------	--

$$X = 3.859$$

Appendix J

EXAMPLE CALCULATION OF THE PXR YIELD EFFECTS DUE TO ROTATING THE CRYSTAL

In this calculation, two important variations are made to the typical PXR yield calculation (see Appendix D). The rotation of the crystal changes the PXR energy at the fixed detector location. This correction is shown in steps 2 and 4. The rotation of the crystal angularly displaces the PXR Bragg condition by twice the rotation angle. This correction is seen in the limits of the integrals shown in steps 3 and 5.

1. Define experimental parameters

$E_0 := 18$	PXR energy [keV]
$R := 3000$	Distance from crystal to detector [mm]
$d_{col} := 3$	Width of collimator [mm]
$L_{up} := \frac{d_{col}}{2} \cdot \frac{1}{R}$	Collimator upper limit of variation in detection solid angle [rad]
$\theta_{ph} := 9.28743 \times 10^{-3}$	Characteristic angle [rad]

2. Increment crystal rotation steps that increase the electron incident angle, ϕ

$a := 1..100$	Index the steps
$\Delta\phi_a := \frac{a}{25} \cdot \frac{\pi}{180}$	Define the rotation step size
$E_{a_{new}} := \frac{4.135 \cdot 10^{-15}}{1000} \cdot c \cdot \frac{\sin(\theta_B(E_0) + \Delta\phi_a)}{d \cdot (1 - \cos(2 \cdot \theta_B(E_0)))}$	Determine PXR energy as a result of the crystal rotation

3. Calculate the PXR flux at the detector of crystal rotation that increases the electron incident angle, ϕ . Assume that the detector sits at the Bragg condition.

For positive $\Delta\phi > 0$

$$\Phi_{a_{new}} := \int_{|2 \cdot \Delta\phi_a| - L_{up}}^{|2 \cdot \Delta\phi_a| + L_{up}} \int_{-L_{up}}^{L_{up}} \frac{(5.809 \cdot 10^{-4}) \cdot F(E_{a_{new}}) \cdot (\chi(E_{a_{new}}))^2 \cdot [\omega(E_{a_{new}}) \cdot [\theta_x^2 \cdot [\cos[2 \cdot (\theta_B(E_0) + \Delta\phi_a)]]^2 + \theta_y^2]]}{2.997 \cdot 10^8 \cdot (\sin(\theta_B(E_{a_{new}})))^2 \cdot [\theta_x^2 + \theta_y^2 + (\theta_{ph})^2]^2} d\theta_y d\theta_x$$

4. Increment crystal rotation steps that decrease the electron incident angle, ϕ

$b := 0..100$	Index the steps
$\Delta\Omega_b := \frac{-b}{25} \cdot \frac{\pi}{180}$	Define the rotation step size
$E_{b_{new}} := \frac{4.135 \cdot 10^{-15}}{1000} \cdot c \cdot \frac{\sin(\theta_B(E_0) + \Delta\Omega_b)}{d \cdot (1 - \cos(2 \cdot \theta_B(E_0)))}$	Determine PXR energy as a result of the crystal rotation

5. Calculate the PXR flux at the detector of crystal rotation that decreases the electron incident angle, ϕ . Assume that the detector sits at the Bragg condition.

For negative $\Delta\phi < 0$

$$\Phi_{\text{new}_b} := \int_{|2 \cdot \Delta\Omega_b| - L_{\text{up}}}^{|2 \cdot \Delta\Omega_b| + L_{\text{up}}} \int_{-L_{\text{up}}}^{L_{\text{up}}} \frac{(5.809 \cdot 10^{-4}) \cdot F(E_{\text{new}_b}) \cdot (\chi(E_{\text{new}_b}))^2 \cdot \left[\omega(E_{\text{new}_b}) \cdot \left[\theta_x^2 \cdot \cos[2 \cdot (\theta_B(E_0) + \Delta\Omega_b)]^2 + \theta_y^2 \right] \right]}{2.997 \cdot 10^8 \cdot \left(\sin(\theta_B(E_{\text{new}_b}))) \right)^2 \cdot \left[\theta_x^2 + \theta_y^2 + (\theta_{\text{ph}})^2 \right]^2} d\theta_y d\theta_x$$

6. Plot the PXR yield as a function of crystal rotation angle [ph/e/9mm²].

APPENDIX K

AN EXAMPLE CALCULATION OF THE DEADTIME/PILEUP CORRECTION TO THE MEASURED COUNT RATES AND THE CORRECTION UNCERTAINTY.

1. Enter measured count rates from spectrum.

$PXR_1 := 10.8$	Count rate from first order peak [cps]
$PXR_2 := 0.8$	Count rate from second order peak [cps]
$Total := 199$	Total count rate for spectrum [cps]
$t := 60$	Count time for spectrum [s]
$f := 400$	LINAC repetition rate [Hz]

2. Calculate the corrected first order peak count rate, CR_1 , and its uncertainty, δCR_1 .

$$CR_1 := \frac{PXR_1 \cdot f}{f - Total}$$

$$\delta CR_1 := \left[\left[\frac{f}{f - ((Total))} \right]^2 \cdot \left[\frac{((PXR_1))}{t} \right] + \left[\frac{f \cdot ((PXR_1))}{[f - ((Total))]^2} \right]^2 \cdot \left[\frac{((Total))}{t} \right] \right]^{.5}$$

3. Calculate the corrected second order peak count rate, CR_2 , and its uncertainty, δCR_2 .

$$CR_2 := f \cdot \left[\frac{PXR_2}{f - Total} - \frac{1}{2} \cdot \left(\frac{PXR_1}{f - Total} \right)^2 \right]$$

$$\delta CR_2 := \left[\left(\frac{f}{f - Total} \right)^2 \cdot \left[\frac{((PXR_2))}{t} \right] + \left[\frac{f \cdot PXR_1}{(f - Total)^2} \right]^2 \cdot \left[\frac{((PXR_1))}{t} \right] + \left[\frac{f}{(f - Total)^2} \cdot \left[PXR_2 + \frac{PXR_1^2}{(f - Total)} \right] \right]^2 \cdot \left[\frac{((Total))}{t} \right] \right]^{.5}$$

4. Calculate the pile-up of two first order photons in the second order peak, $Pile$, and its uncertainty, $\delta Pile$.

$$Pile := \frac{f}{2} \cdot \left(\frac{PXR_1}{f - Total} \right)^2$$

$$\delta Pile := \left[\left[\frac{f \cdot PXR_1}{(f - Total)^2} \right]^2 \cdot \left[\frac{((PXR_1))}{t} \right] + \left[\frac{f \cdot (PXR_1)^2}{(f - Total)^3} \right]^2 \cdot \left(\frac{Total}{t} \right) \right]^{.5}$$

5. Calculate the corrected total count rate, TR .

$$TR := f \cdot \ln \left[\frac{f}{f - ((Total))} \right]$$

APPENDIX L

TABULATED PXR DATA AND THE PREDICTED EFFECTS OF MOSAICITY AND ELECTRON BEAM MULTIPLE SCATTERING

This appendix tabulates the PXR data, experimental conditions, and the calculated electron multiple scattering from electron interactions with the PXR target crystal, the LINAC output window, and the air pathway from the window to the crystal. The standard deviation of the electron scattering is used to broaden the PXR photon distribution. Calculations are shown for the photon absorption in air from the crystal to the detector and for the detector deadtime correction and efficiency. The tabulated data is present in the landscape page format. For a given experiment, the data runs across the two tabulated pages in this appendix.

															</								

Note 1

Small Crystal

Note 2

WaterBucket Current Measurement/AI Window

	Comments	Crystal	Measured Rates Error	Corrected/Air-Dead Data Corrected Rate	Theory Rates Error 10% current	PXR Theory E Predicted CPS E	Yield [photon/e/ 9 mm ²] electron sigma from crystal/window/air [rad]	Air path sigma [rad]	Air path distance [cm]	PXR Theory D Predicted CPS D	Yield [photon/e/ 9 mm ²] electron sigma from crystal and window [rad]		PXR Theory C Predicted CPS C	Yield [photon/e/ 9 mm ²] electron sigma from crystal [rad]		PXR Theory B Predicted CPS B
	Note 1	C002	129.2	1730.6	73.5	734.9	6.647E-08	0.0462	5.00	745.0	6.739E-08	0.0456	755.4	6.833E-08	0.0450	3009.6
	Note 1	Cu222	1.1	13.0	0.9	9.1	1.988E-11	0.0878	8.00	9.1	2.000E-11	0.0873	9.2	2.008E-11	0.0870	176.3
	Note 1	LiF222	2.1	23.0	31.8	317.9	3.812E-10	0.0342	8.00	332.3	3.984E-10	0.0329	342.8	4.111E-10	0.0320	1507.1
	Note 1	LiF400	20.3	311.4	13.9	138.5	2.053E-10	0.0342	8.00	144.8	2.146E-10	0.0329	149.4	2.214E-10	0.0320	667.7
	Note 1	LiF400	24.5	382.1	48.7	487.0	2.025E-10	0.0269	8.00	688.2	2.862E-10	0.0251	719.0	2.991E-10	0.0240	1794.2
		Si111	65.6	639.5	200.2	2002.2	2.043E-09	0.0452	5.00	2035.5	2.077E-09	0.0446	2069.6	2.112E-09	0.0440	13385.9
		Si220	22.1	238.7	142.9	1429.2	1.985E-09	0.0209	8.00	2315.4	3.216E-09	0.0186	2475.4	3.438E-09	0.0170	4353.0
		Si400	46.4	591.1	83.2	832.4	1.927E-10	0.0278	8.00	888.5	2.057E-10	0.0261	927.7	2.147E-10	0.0250	3026.2
		Si440	5.9	90.0	35.4	353.7	1.935E-10	0.0217	8.00	388.1	2.123E-10	0.0195	413.9	2.264E-10	0.0180	1072.9
		Si440	9.2	132.2	169.5	1695.3	1.999E-10	0.0217	8.00	1860.2	2.194E-10	0.0195	1983.7	2.339E-10	0.0180	5152.1
	Note 1	W222	1.0	9.7	0.5	5.4	2.311E-11	0.1714	8.00	5.4	2.313E-11	0.1712	5.4	2.314E-11	0.1710	104.0
		LiF200	52.3	841.9	25.2	251.7	3.820E-09	0.0597	20.32	260.2	3.948E-09	0.0575	262.3	3.980E-09	0.0570	1421.7
		LiF220	15.6	187.2	13.2	132.1	1.651E-09	0.0331	20.32	152.6	1.907E-09	0.0290	158.3	1.979E-09	0.0280	460.0
		LiF200	25.2	388.6	151.0	1510.4	3.820E-09	0.0597	20.32	1561.4	3.948E-09	0.0575	1573.9	3.980E-09	0.0570	8563.6
		LiF200	20.2	302.3	102.0	1019.5	3.820E-09	0.0597	20.32	1054.0	3.948E-09	0.0575	1062.4	3.980E-09	0.0570	5780.4
		LiF220	12.0	134.2	50.6	506.4	6.663E-10	0.0348	20.32	579.1	7.619E-10	0.0309	598.1	7.870E-10	0.0300	2359.9
		LiF400	9.0	129.7	13.3	133.0	1.750E-10	0.0437	20.32	131.2	1.727E-10	0.0407	134.0	1.763E-10	0.0400	778.9
		LiF220	61.6	842.7	17.9	179.1	1.599E-09	0.0341	25.40	213.9	1.910E-09	0.0290	220.7	1.971E-09	0.0280	643.3
		LiF220	35.0	417.7	21.1	211.4	1.602E-09	0.0341	25.40	252.6	1.913E-09	0.0290	260.1	1.971E-09	0.0280	758.9
		LiF220	47.9	641.9	33.2	331.8	8.295E-10	0.0349	25.40	393.0	9.825E-10	0.0300	407.6	1.019E-09	0.0290	1434.3
	Note 2	LiF220	38.6	452.7	52.0	520.4	1.121E-09	0.0458	25.40	575.7	1.241E-09	0.0421	914.4	1.971E-09	0.0280	2660.8
	Note 2	LiF220	31.4	359.0	51.9	519.2	1.119E-09	0.0458	25.40	575.7	1.241E-09	0.0421	914.4	1.971E-09	0.0280	2657.7
	Note 2	Si220	15.4	202.3	32.2	321.8	1.149E-09	0.0401	25.40	367.8	1.313E-09	0.0358	750.2	2.679E-09	0.0170	1366.4
	Note 2	Si400	9.6	91.7	16.2	161.9	5.784E-10	0.0504	25.40	176.3	6.296E-10	0.0471	251.8	8.993E-10	0.0350	939.9
		Si220	44.6	439.9	96.5	964.6	2.412E-09	0.0259	25.40	1295.5	3.239E-09	0.0186	1385.1	3.463E-09	0.0170	2442.0
		Si220	104.1	886.3	106.1	1061.1	2.412E-09	0.0259	25.40	1425.1	3.239E-09	0.0186	1523.6	3.463E-09	0.0170	2686.2
		Si220	37.2	397.8	54.0	540.2	2.412E-09	0.0259	25.40	725.5	3.239E-09	0.0186	775.6	3.463E-09	0.0170	1367.5