Reciprocal Space Phase Gradient Neutron Imaging

by

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Submitted to the Physics Department
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Abstract

Perfect crystal real space imaging has limitations in its resolution imposed by position-sensitive detectors. The disadvantage, its limited resolution, of a position-sensitive detector can be overcome by replacing the conventional detector with an area detector and moving to reciprocal space. Reciprocal space imaging is proposed in this thesis with the state-of-the-art neutron interferometry at National Institute of Standard and Technology. An aluminium wedge produces various phase gradients and a specially designed sample is introduced as a test subject. Superposition of the waves from the sample beam path and the gradient wedge beam path creates an interferogram that suggests an inhomogeneous phase distribution. The result shows the existence of spatially encoded phase gradients, even though imaging was unsuccessful. A next generation design of reciprocal space imaging is proposed in the conclusion.

Thesis Supervisor: David G. Cory
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Chapter 1

Introduction

Neutrons are especially good sources to explore the structure of materials and they have offered several approaches to phase contrast imaging. [11][13][3] The interesting examples use a perfect crystal interferometer. However, these methods obtain spatial resolution via a 2-dimensional position sensitive detector, which has the disadvantage of very limited spatial resolution.

We showed that a new approach to neutron imaging is possible by moving the experimental measurement to reciprocal space in analogy to Nuclear Magnetic Resonance (NMR) imaging. Here the spatial information is encoded in the phase of the spin and the various Fourier components of the material property are directly read out. The spatially resolved detector is thus replaced with an area detector since the only information required is the contrast as a function of the k-vector, which describes the spatial rate of change of the spin’s phase.

Encoding a spatially distributed phase gradient is the core of this new approach. Previously, we proposed that this phase encoding could be done by a magnetic gradient coil.[8] While our goal is to control the neutron spin degrees of freedom using the gradient field, we can show that the gradient phase encoding combined with neutron interferometry produces a new method of neutron imaging called Reciprocal Space Neutron Imaging. This chapter briefly reviews two imaging methods and discusses the advantages and disadvantages of reciprocal space imaging.
1.1 Real Space Imaging

Neutrons are attenuated mostly by light materials like hydrogen atoms or some selected isotopes. Therefore, it has been possible to see what could not be observed by other radiographic sources. For example, biological crystallography is one of the applications made possible because neutrons can analyze the distribution of hydrogen atoms, which take a large portion of biomacromolecules.[10] Other applications of neutron imaging include the non-destructive testing of explosive devices, nuclear materials and aircraft components.[5]

A plate type of a neutron detector has been used for many types of imaging experiments.[6][7][10] An electronic neutron imaging camera system, which utilizes a plate neutron scintillator, is widely used for thermal neutrons in non-destructive testing. This system mainly consists of two parts.[12][5] The scintillator emits photons when a neutron strikes it. Then, photons are detected by a CCD camera, which visualizes where the particles were detected. While these position-sensitive detectors are used mostly for two-dimensional imaging, the tomography concept involving a position-sensitive detector has also been proposed for perfect crystal neutron interferometry.[3]

The real space profile of the sample $P(x, y)$, which represents absorption of neutrons or even phases of neutrons when combined with a neutron interferometer, is projected to the CCD camera.(Fig. 1-1) Then, an external display unit only transforms the signal from CCD. Since the image profile is recorded in spatial coordinate, no extra processing of an imaging data is required to visualize the image.

Generally, two-dimensional detectors have shown resolutions of $0.2 \sim 0.5$ mm.[15][12][9][5] But currently existing position sensitive detectors have resolution limitations imposed by the scintillator, and the resolutions are fixed by the its characteristic.
1.2 Reciprocal Space Imaging

In reciprocal space imaging, the spatial information is encoded in the phase of the neutron, and the Fourier components of the material property are directly measured. Therefore, the image profile of a sample, $P(x, y)$, is recorded in k-space:

$$I(\vec{k}) = \frac{1}{(2\pi)^2} \int P(x, y) e^{i\vec{k} \cdot \vec{r}} d^2 \vec{r}. \quad (1.1)$$

Thus, the spatially resolved detector is replaced with an area detector since the only information required is the intensity of the superposed wave as a function of the k-vector, which describes the spatial rate of change of the neutron’s phase. The advantage of reciprocal space imaging is that the resolution of the image is now governed by the k-vector, the gradient. Its resolution gets smaller as one achieves a higher gradient. And the resolution is given by the Nyquist theorem:

$$\Delta x = \frac{\pi}{k_{max}}. \quad (1.2)$$
Once the intensity profile $I(\mathbf{k})$ is obtained for a complete set of wave-numbers, a real space image is reconstructed via a Fourier transformation:

$$P(x, y) = \int I(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{r}} d^2 \mathbf{k}.$$  

(1.3)

Since neutron interferometry shows high sensitivity to a neutron’s phase, a perfect crystal interferometer is considered to be an ideal tool to control and read out the phase of a neutron. In following chapters, I will describe in detail how reciprocal space imaging is done with a perfect crystal.
Chapter 2

Fundamentals of Lattice

2.1 Lattice

Since the core requirement of the experiment is a perfect crystal, it is important to understand properties of crystals. Basic knowledge of the Bravais lattice is presented at the beginning, and several terminologies of solid state physics are defined. Finally, basic diffraction theory is introduced with the Ewald sphere. The next chapter will cover diffraction theory in more detail.

2.1.1 Bravais Lattice

An ideal crystal structure is constructed by periodic arrays of atoms. We can express the positions of atoms, \( \vec{r} \), using a formula with integers \( u_1, u_2 \) and \( u_3 \) and basis vectors \( \vec{a}_1, \vec{a}_2 \) and \( \vec{a}_3 \) (Fig. 2-1):

\[
\vec{r} = \vec{r} + u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3.
\]  

(2.1)

Here, vector \( \vec{r} \) is any atom’s position in the crystal. A set of integers \( u_1, u_2 \) and \( u_3 \) now defines a lattice. Combined with the basis vector, it generates a crystal structure.(Fig. 2-1) We can also view the lattice structure as a set of translation operations done to the original position \( \vec{r} \). Therefore, we define a translation operation of a lattice as

\[
\vec{T} = u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3.
\]  

(2.2)
The lattice which can be made from this translation operation is called Bravais lattice. Usually, the term Bravais lattice is used when we refer to certain types of lattice. For example, there are five different lattice systems for the two-dimensional lattice case, which are symmetric under specific rotations. (Fig. 2-2)

### 2.1.2 Diamond Structure

There are fourteen different three-dimensional lattice types. The diamond lattice consists of the two face-centered cubic (fcc) Bravais lattices. Therefore, it shows the tetrahedral bond arrangement. The perfect crystal which is used for the experiment in this thesis is also made from an element that shows the diamond structure, Si. (Fig. 2-3)
Figure 2-2: Five Bravais lattice types are shown for the two-dimensional lattice case.
Figure 2-3: Diamond structure. A diamond lattice consists of two fcc Bravais lattices displaced by $\frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$.

### 2.1.3 Reciprocal Lattice

A reciprocal lattice is defined as a set of all wave vectors that shows periodicity of a given Bravais lattice. Consider a plane wave $e^{i\mathbf{r} \cdot \mathbf{k}}$ and a point $\mathbf{R}$ of a Bravais lattice. Then, specific wave vectors expressed as $\mathbf{H}$ show periodicity corresponding to $\mathbf{H}$:

$$e^{i\mathbf{R} \cdot (\mathbf{r} + \mathbf{H})} = e^{i\mathbf{R} \cdot \mathbf{r}}.$$  \hspace{1cm} (2.3)

In other words,

$$e^{i\mathbf{H} \cdot \mathbf{R}} = 1.$$  \hspace{1cm} (2.4)

For example, the primitive vectors for an fcc lattice are

$$\vec{a}_1 = \frac{1}{2}a(\hat{y} + \hat{z}); \quad \vec{a}_2 = \frac{1}{2}a(\hat{x} + \hat{z}); \quad \vec{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y}),$$  \hspace{1cm} (2.5)

and the reciprocal lattice vectors can be found as

$$\vec{b}_1 = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}); \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}); \quad \vec{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z}).$$  \hspace{1cm} (2.6)
2.1.4 Lattice Plane

A plane can be found with three Bravais lattice points that are not aligned on a same line (non-collinear points). Since the reciprocal lattice vector is a vector which satisfies Eq. 2.4, for any family of lattice planes there exist reciprocal lattice vectors that are perpendicular to the lattice planes. The shortest reciprocal wave vector should be $2\pi/d$ if lattice planes are separated by a distance $d$. (Fig. 2-4)

One way to express the lattice plane is by using the Miller indices, which are the integer coordinates of the shortest reciprocal lattice vector normal to that plane. Generally, lattice planes are described by their Miller indices in parentheses, i.e., $(h,k,l)$. Since the Miller indices are all integers representing the shortest possible vector, $h$, $k$, and $l$ cannot have a common factor. With this rule in mind, the Miller indices whose lattice plane intersects with primitive vector axes at points $x_1\vec{a}_1$, $x_2\vec{a}_2$, 

---

Figure 2-4: One example of lattice planes for a fcc Bravais lattice. The shortest $\vec{K}$ is $\vec{K} = 2\pi/d \hat{n}$. 
and $x_3 \vec{a}_3$, can be easily found by using the relation:

$$h : k : l = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}. \quad (2.7)$$

Another convention for describing a lattice plane is using the direct lattice coordinate. If the lattice plane intersects with $n_1 \vec{a}_1$, $n_2 \vec{a}_2$, and $n_3 \vec{a}_3$, the plane is said to be in the $[n_1 n_2 n_3]$ direction.

### 2.2 Ewald Sphere

#### 2.2.1 Bragg Law

Consider lattice planes spaced $d$ apart as in Fig. 2-5. Bragg law states that constructive interference of the diffracted rays from the lattice planes occurs when the path difference is an integer multiple of wavelength $\lambda$:

$$2d \sin \theta = n \lambda. \quad (2.8)$$

#### 2.2.2 Laue Condition

Laue condition is another way of describing the diffraction of rays from lattice planes. According to the Laue description, every point in the lattice reradiates incident rays in all directions. But when a constructive condition is imposed and satisfied, a sharp peak of diffracted beam intensity will be observed only in one specific direction $\theta$. When incident ray of wave vector $\vec{k}$ is scattered at an angle, $\theta'$, constructive interference occurs only if the following equation is satisfied (Fig. 2-6):

$$d \cos \theta + d \cos \theta' = m \lambda. \quad (2.9)$$
Figure 2-5: Lattice planes are separated by $d$. The incident beam has an oblique angle of $\theta$.

Figure 2-6: Two scattering points and a reciprocal vector $\vec{K}$ satisfying Laue condition.
We can rewrite $\cos \theta$ and $\cos \theta'$ using vectors:

$$\vec{d} \cdot (\vec{k} - \vec{k}') = 2\pi m. \tag{2.10}$$

For the constructive interference to be true for all the incident rays, Eq. 2.10 must hold for any Bravais lattice vector $\vec{R}$ so that the equation,

$$\vec{R} \cdot (\vec{k} - \vec{k}') = 2\pi m, \tag{2.11}$$

is satisfied. Now using Eq. 2.4, the Laue condition becomes

$$\vec{H} = \vec{k}' - \vec{k}. \tag{2.12}$$

Since the vector $\vec{H}$ is the shortest reciprocal vector, $2\pi/d\hat{n}$, multiplied by an integer, $n$, it follows from Fig. 2-6 that the relation,

$$2k \sin \theta = \frac{\pi n}{d}, \tag{2.13}$$

is true in general. Thus, Bragg law follows from the Laue condition.

### 2.2.3 Ewald Sphere

The Laue condition imposes a relation among three vectors $\vec{k}_0$, $\vec{k}$ and $\vec{H}$. They must form a triangle with two identical sides as shown in Fig. 2-7.

If a sphere is constructed with the center at the origin of $\vec{k}_0$ and $|\vec{k}_0|$ as a radius, the diffracting Laue condition is satisfied only if the two end points of vector $\vec{H}$ are on the surface of the sphere.(Fig. 2-8) This sphere in reciprocal space is called the Ewald sphere. Once we know the reciprocal vector $\vec{H}$ of the lattice plane we are interested in, the diffracted wave vector $\vec{k}$ can be determined from the Ewald sphere.
Figure 2-7: Vector diagram of Laue condition.

Figure 2-8: Three vectors constrained by the Laue condition. $\vec{k}_0$ and $\vec{k}$ are incident and diffracted wave vectors, respectively, and $\vec{H}$ is a reciprocal lattice vector.
Chapter 3

Waves in Crystals

Until the state-of-the-art technology called a perfect crystal became available it was not easy to see neutron waves interfering with each other because of the extremely short coherence length of neutron waves. It was a perfect silicon crystal that made it possible to split and properly recombine neutron waves coherently enough to see quantum mechanical interference of neutron waves. This chapter reviews theories necessary to understand the interference in a perfect crystal in terms of quantum mechanical wave functions.

3.1 Waves inside a Crystal

In a relatively thick crystal, a diffracted beam is backscattered and then diffracted again. This process of consecutive diffraction is called dynamical diffraction. Many parts of this section refer to well known articles such as *The Dynamical Diffraction Theory of X-ray* by Batterman(1964)[4]. An article by Arthur and Shull[2] is another useful reference for the case of the dynamical diffraction of a neutron.

3.1.1 Dispersion Relation

Let us assume that the incident monochromatic wave can be denoted as $A_0 e^{i\vec{k}_0 \cdot \vec{r}}$ with $\vec{k}_0$ oriented at or near Bragg condition for the lattice planes. Then, inside the crystal
a Schrödinger equation with the periodic lattice potential $v(\vec{r})$ holds:

$$
(\nabla^2 + \hbar^2 \kappa_0^2) \psi(\vec{r}) = v(\vec{r}) \psi(\vec{r}), \quad \text{with}
$$

$$
v(\vec{r}) = \frac{2m}{\hbar^2} V(\vec{r}) = \text{scaled periodic potential}.
$$

In this Schrödinger equation, the periodic potential inside the crystal can be decomposed into several important Fourier components because a perfect crystal is a periodic system. In general, a periodic potential is written as

$$
V(\vec{r}) = \frac{2\pi \hbar^2}{m} \sum_j b_j \delta(\vec{r} - \vec{r}_j),
$$

which is often referred to a periodic Fermi pseudo-potential. Thus, a Fourier series form of this potential may be written as

$$
V(\vec{r}) = \sum_{H} V_{H} e^{iH \cdot \vec{r}}.
$$

The coefficients of this potential can be calculated using a dirac-delta function produced when integrating over a unit cell:

$$
\sum_{H'} V_{H'} e^{iH' \cdot \vec{r}} = V(\vec{r})
$$

$$
\frac{1}{V_{\text{cell}}} \sum_{H'} \int V_{H'} e^{iH' \cdot \vec{r}} e^{iH \cdot \vec{r}} d^3 \vec{r} = \frac{1}{V_{\text{cell}}} \int V(\vec{r}) e^{iH \cdot \vec{r}} d^3 \vec{r}
$$

$$
V_{H} = \frac{1}{V_{\text{cell}}} \int \frac{2\pi \hbar^2}{m} \sum_j b_j \delta(\vec{r} - \vec{r}_j) e^{iH \cdot \vec{r}} d^3 \vec{r}
$$

$$
= \frac{2\pi \hbar^2}{m V_{\text{cell}}} \sum_j b_j e^{iH \cdot \vec{r}_j}.
$$

And we define the structure factor for the Bravais lattice as

$$
F_{H} = \sum_j b_j e^{iH \cdot \vec{r}_j}.
$$

25
We often use potentials like Eq. 3.1, in which case the relation between the structure factor and Fourier coefficient is given by

\[ v_{\mathbf{h}} = \frac{4\pi}{V_{\text{cell}}} F_{\mathbf{h}}. \]  

(3.6)

Since we are working in Laue condition, only \( v_{\pm \mathbf{h}} \) and the mean potential \( v_0 \) are significant. The potential couples \( \vec{K}_0 \) and diffracted wave vector through the Bragg relation or equivalently Laue condition,

\[ \vec{K}_{\mathbf{h}} = \vec{K}_0 + \vec{H}. \]  

(3.7)

Note that the \( \vec{K}_0 \) is going to be slightly different from \( \vec{k}_0 \) due to the refraction of the crystal medium. The field inside the crystal then, can be given by the sum of two wave functions: forwarding and diffracting waves,

\[ \psi(\mathbf{r}) = \psi_0 e^{i \vec{K}_0 \cdot \mathbf{r}} + \psi_{\mathbf{H}} e^{i \vec{K}_{\mathbf{h}} \cdot \mathbf{r}}. \]  

(3.8)

We use Eq. 3.8 as a solution to the Schrödinger equation. Then,

\[ (\nabla^2 + k_0^2)[\psi_0 e^{i \vec{K}_0 \cdot \mathbf{r}} + \psi_{\mathbf{H}} e^{i \vec{K}_{\mathbf{h}} \cdot \mathbf{r}}] = v(\mathbf{r})[\psi_0 e^{i \vec{K}_0 \cdot \mathbf{r}} + \psi_{\mathbf{H}} e^{i \vec{K}_{\mathbf{h}} \cdot \mathbf{r}}]. \]  

(3.9)

Now multiplying \( e^{-i \vec{K}_0 \cdot \mathbf{r}} \) by Eq. 3.9 and integrating over a unit cell results in

\[ -K_0^2 \psi_0 \int d\mathbf{r} + K_0^2 \psi_0 \int d\mathbf{r} - K_H^2 \psi_{\mathbf{H}} \int e^{i \vec{K}_{\mathbf{h}} \cdot \mathbf{r}} e^{-i \vec{K}_0 \cdot \mathbf{r}} d\mathbf{r} + k_0^2 \psi_{\mathbf{H}} \int e^{i \vec{K}_{\mathbf{h}} \cdot \mathbf{r}} e^{-i \vec{K}_0 \cdot \mathbf{r}} d\mathbf{r} \]  

(3.10)

\[ = v_0 \psi_0 \int d\mathbf{r} + v_0 \psi_0 \int e^{i \vec{K}_0 \cdot \mathbf{r}} e^{-i \vec{K}_0 \cdot \mathbf{r}} + v_{\mathbf{H}} \psi_{\mathbf{H}} \int e^{i \vec{H} \cdot \mathbf{r}} d\mathbf{r} + v_{\mathbf{H}} \psi_{\mathbf{H}} \int e^{i \vec{H} \cdot \mathbf{r}} e^{-i \vec{K}_0 \cdot \mathbf{r}} d\mathbf{r} + v_{-\mathbf{H}} \psi_{-\mathbf{H}} \int e^{-i \vec{H} \cdot \mathbf{r}} d\mathbf{r} + v_{-\mathbf{H}} \psi_{-\mathbf{H}} \int e^{-i \vec{H} \cdot \mathbf{r}} e^{-i \vec{K}_0 \cdot \mathbf{r}} d\mathbf{r}. \]

Since there is a volume integral involved, we divide both sides by the unit cell volume. And to make use of the fact that the integral of \( e^{i \vec{H} \cdot \mathbf{r}} \) over a unit cell is zero for the periodic lattice, we rewrite all the exponentials using \( \vec{H} \cdot \mathbf{r} \). After dividing by a unit
cell volume, $V_{cell}$, we have

$$-K_0^2 \psi_0 + k_0^2 \psi_0 - K_H^2 \psi_H \frac{1}{V_{cell}} \int e^{i \vec{H} \cdot \vec{r}} d\vec{r} + k_0^2 \psi_H \frac{1}{V_{cell}} \int e^{i \vec{H} \cdot \vec{r}} d\vec{r}$$ (3.11)

$$= \psi_0 + v_H \psi_0 \frac{1}{V_{cell}} \int e^{i \vec{H} \cdot \vec{r}} d\vec{r} + v_H \psi_H \frac{1}{V_{cell}} \int e^{i \vec{H} \cdot \vec{r}} d\vec{r}$$

$$+ v_{-H} \psi_0 \frac{1}{V_{cell}} \int e^{-i \vec{H} \cdot \vec{r}} d\vec{r} + v_{-H} \psi_H \frac{1}{V_{cell}} \int d\vec{r}.$$ (3.12)

Here, Eq. 3.7 was used to rewrite exponentials in terms of $\vec{H} \cdot \vec{r}$. Since integrals of $e^{i \vec{H} \cdot \vec{r}}$ over a unit cell equals zero for the periodic lattice, we finally have

$$-\psi_0 K_0^2 + k_0^2 \psi_0 = \psi_0 + v_{-H} \psi_H. \quad (3.13)$$

Introducing $K^2 = k_0^2 (1 - \frac{V_0}{E_0})$, where $E_0$ is the incident neutron kinetic energy, leads us to

$$(K^2 - K_0^2) \psi_0 - v_{-H} \psi_H = 0. \quad (3.14)$$

Similarly, we multiply $e^{-i \vec{H} \cdot \vec{r}}$ by Eq. 3.9 and integrate over a unit cell to obtain a second equation,

$$-v_H \psi_0 + (K^2 - K_H^2) \psi_H = 0. \quad (3.15)$$

For the amplitudes of wave functions to have non-trivial solutions, the determinant should be zero:

$$(K^2 - K_0^2)(K^2 - K_H^2) = v_H v_{-H}. \quad (3.16)$$

Since $K$, $K_0$ and $K_H$ are not much different from $k_0$ we can write approximately

$$K + K_0 \simeq 2k_0, \quad K + K_H \simeq 2k_0. \quad (3.17)$$

Then Eq. 3.15 can be written, to a very good approximation,

$$(K - K_0)(K - K_H) = v_H v_{-H}/4k_0^2. \quad (3.18)$$
Figure 3-1: Q is the center of the Ewald circle. The incident wave vector $\vec{k}_0$ is different from the incident wave vector inside the crystal, $\vec{K}$. Since the difference between $\vec{K}_O$ and $\vec{K}$ is too small, it is hard to separate these vectors from this figure.

3.1.2 Ewald Sphere

In the previous chapter, I briefly explained the Ewald sphere description of diffraction. With wave vectors $\vec{K}_O, \vec{K}_H$ and $\vec{H}$, we can draw a sphere centered at $Q$ with forward diffracted wave directing $O$ and diffracted beam directing $H$. Now our goal is to find solutions of Eq. 3.17. To help understand the process of finding solutions, we are going to use a circle instead of a sphere. (Fig. 3-1) The dispersion relation (Eq. 3.15) defines a trajectory where the Laue condition can be satisfied inside the crystal. Since the dispersion equation is a quadratic equation for $K$, there should be four general solutions. The points that satisfy Eq. 3.17 create a hyperbola around the point $Q$. (Fig. 3-2) Depending on which side of hyperbola the solutions are, we name them as $\alpha$ branch solutions and $\beta$ branch solutions. There are two solutions respectively on each side of hyperbola. One example of solutions is given in Fig. 3-2. When the solution is chosen to be at $M$, one can calculate the length of $MM'$ from Eq. 3.17, and this is called a characteristic inverse length. Since $MC' = MC, K - K_O = K - K_H = (v_H v_{-\vec{H}}/4k_0^2)^{1/2}$. Furthermore, with the Bragg angle $\theta_B$, we can calculate $MQ$ to be
Figure 3-2: The center region around Q is described on the left in detail. Because P is very close to Q, PH \parallel MH and PO \parallel MO can be assumed.

\[(v_H v_{-H}/4k_0^2)^{1/2} \sec \theta_B.\] Then,

\[MM' = (v_H v_{-H})^{1/2}/k \cos \theta_B \quad (\because \ MM' = 2MQ). \quad (3.18)\]

Here, we assumed that solutions are not much different from \( \vec{K}_O \) and \( \vec{K}_H \). Then, the spheres with radius of \( \vec{K}_O \) and \( \vec{K}_H \) viewed at the loci of the focal plane of the hyperbola can be approximated to planes. The asymptotic lines in this figure represent these approximated planes. This approximation can be confirmed to be valid by simple calculation as follows.

Let us calculate the characteristic length of a silicon crystal starting from Eq. 3.6. The structure factor is given by \( F_{\vec{H}} = \sum_j b e^{i\vec{H} \cdot \vec{r}_j} \) with lattice vectors \( \vec{r}_j = x_j \vec{a}_1 + y_j \vec{a}_2 + z_j \vec{a}_3 \), reciprocal vector \( \vec{H} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \) and a coherent scattering length \( b \). Since a diamond lattice is a lattice with two basis vectors at \( \vec{d}_1 = 0 \) and \( \vec{d}_2 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z}) \), four lattice points coming from each fcc lattice consist of the structure factor. Each fcc structure had identical atoms at \( (x_j y_j z_j) = 000, 0\frac{1}{2} \frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0 \). Thus
lattice points of eight atoms consisting of diamond structure of a silicon crystal are

\[ 000, 011, 101, 110, 111, 133, 311, 331. \]

For (111) plane of a silicon crystal, we have

\[
F_{111} = b \sum_j e^{i2\pi(x_j + y_j + z_j)} 
\]

\[
= b(e^0 + e^{i2\pi} + e^{i2\pi} + e^{i2\pi} + e^{i2\pi} + e^{i2\pi} + e^{i2\pi} + e^{i2\pi}) 
\]

\[
= b(5 + 2i).
\]

The coherence scattering length of Si is about 4 fm[1], which leads \( F_H \) to be, approximately, \( 10^{-14} \) m. A unit cell volume of silicon is about \( (5.43 \times 10^{-10})^3 \) since the lattice constant of silicon is 5.43 Å. Thus, we estimate the value of \( v_H \) to be around \( 10^{15} \) m\(^{-1}\). Thermal neutrons of wavelength of 2.7 Å has a wave vector of the order of \( 10^{10} \) m\(^{-1}\), which is also the magnitude of \( Q_O \) or \( Q_H \). But the separation \( MM' \) given by Eq. 3.18 is of the order of \( 10^4 \) m\(^{-1}\). Therefore, it is true that we are looking at a very small portion of the spheres crossing at \( Q \), and Fig. 3-2 has been greatly enlarged to visualize different solutions.

### 3.1.3 Four Wave Functions

We have seen that one incident wave generates four different waves with four different wave vectors \((\vec{K}_O, \vec{K}_O, \vec{K}_H, \vec{K}_H)\). Then a total wave field inside the crystal is

\[
\psi(\vec{r}) = \psi^\alpha_O e^{iK^\alpha_O \cdot \vec{r}} + \psi^\beta_O e^{iK^\beta_O \cdot \vec{r}} + \psi^\alpha_H e^{iK^\alpha_H \cdot \vec{r}} + \psi^\beta_H e^{iK^\beta_H \cdot \vec{r}} \quad (3.20)
\]

We are going to find coefficients of this wave function using Ewald sphere geometry. From Eq. 3.13 and Eq. 3.14 we can define the amplitude ratio of total wave field(Eq. 3.20):

\[
\frac{\psi^\alpha_H}{\psi^\alpha_O} = K - \frac{\nu_H}{\nu_O} = \frac{\nu_H}{K - \alpha_H} \quad (3.21)
\]
where vector notations are dropped for convenience. With the boundary condition of the wave near the entrance surface:

\begin{align*}
\psi_O + \psi_O^\beta &= A_0 \\
\psi_H + \psi_H^\beta &= 0,
\end{align*}

(3.22)

it is possible to express all four coefficients with a constant $A_0$ as long as we know $K - K_{O,H}$. In Fig. 3-3, these quantities are simply the distances between points on the hyperbola and asymptotic lines ($\overline{AC}_O$ or $\overline{AC}_H$). Here, the incident beam enters at point L at an exact Bragg angle. When the beam is slightly off from the Bragg angle by $\Delta \theta$, it enters from point P. Since the amplitude of the incident wave vector $k_0$ is still the same, P is on the arc of a circle with radius of $LO$. Inside the crystal, the wave vector changes but the tangential component should be conserved by the boundary conditions. Therefore, point A on the dispersion surface is determined by the normal surface vector of the crystal. However, the outgoing wave vector from the crystal should conserve energy as well. Then, $L'$ can be found by drawing a circle with radius of $\overline{LH}$. Although $H_1$, $H_2$, $H_3$, and $H$ look like separate points, they all converge at $H$ (the same for $O$, $O_1$, $O_2$) as can be seen in Fig. 3-4. Now our goal is to find the distance $K - K_O$ and $K - K_H$ from the Ewald sphere. From Fig. 3-3,

\[ \angle LOP = \Delta \theta = \overline{LP}/k_0. \]  

(3.23)

Before we go further, $\angle P'L'P$ needs to be expressed in terms of the Bragg angle $\theta_B$. From the geometry, following relations are satisfied:

1. $\angle LPM = \theta_B \therefore \angle LPN = \theta_B$
2. $\angle P'L'P = 2\theta_B \therefore \overline{LP}' || N\overline{P}$

Then, $\overline{PH}$ can be rewritten as

\[ \overline{PH} = \overline{PP}' + \overline{PP}' + \overline{PP}' + \overline{LH} \]  

(3.24)

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Figure 3-3: Close look at the dispersion surface. An incident beam which is slightly off from the exact Bragg angle enters at point P.

Figure 3-4: Because the dispersion surface is extremely small compared to the Ewald sphere of a radius of $k_0$, $\overline{LH}$, $\overline{PH_1}$, $\overline{LH_2}$, $\overline{AH_3}$ may be viewed as parallel lines, and they converge at $H$. (the same with $\overline{LO}$, $\overline{AO_1}$, $\overline{PO_2}$)
\[ \mathbf{L} \mathbf{P} \sin 2\theta_B + k_0. \]

We also know that \( K_O = k_0 - \mathbf{P} \mathbf{A} \cdot \hat{s}_O \) and \( K_H = \mathbf{P} \mathbf{H} - \mathbf{P} \mathbf{A} \cdot \hat{s}_H \) where \( \mathbf{P} \mathbf{A} \) is the vector that is normal to the crystal surface and gives refraction to the original wave vector \( k_0 \). Directions to \( O \) and \( H \) are represented by \( \hat{s}_O \) and \( \hat{s}_H \) respectively. If the Laue condition is satisfied, \( \mathbf{K}_O + \mathbf{K}_H = \mathbf{H} \), vectors form an isosceles triangle. Thus, \( \mathbf{P} \mathbf{A} \cdot \hat{s}_O = \mathbf{P} \mathbf{A} \cdot \hat{s}_H \) when \( \theta = \theta_B \). As a result, \( K_H \) can be expressed with \( K_O \) and \( \theta_B \):

\[ K_H = K_O - k_0 \Delta \theta \sin 2\theta_B. \]  \hspace{1cm} (3.25)

Let’s denote the distance \( K - K_O \) and \( K - K_H \) as \( \xi_O \) and \( \xi_H \) so that

\[ \xi_O = K - K_O, \]  \hspace{1cm} (3.26)
\[ \xi_H = K - K_H = K - K_O + k_0 \Delta \theta \sin 2\theta_B = \xi_O + k_0 \Delta \theta \sin 2\theta_B. \]

Using the dispersion relation Eq. 3.17, we finally have a second order equation for \( \xi_O \):

\[ \xi_O^2 + k_0 \Delta \theta \sin 2\theta_B \xi_O - |\nu_H|^2 = 0. \]  \hspace{1cm} (3.27)

Solving this equation for \( \xi_O \) gives

\[ \xi_O = \frac{1}{2}(-k_0 \Delta \theta \sin 2\theta_B \pm \sqrt{(k_0 \Delta \theta \sin 2\theta_B)^2 + 4|\nu_H|^2}) \]  \hspace{1cm} (3.28)
\[ = \frac{1}{2} \left(-k_0 \Delta \theta \sin 2\theta_B \pm 2|\nu_H| \sqrt{\left(\frac{k_0 \Delta \theta \sin 2\theta_B}{2|\nu_H|}\right)^2 + 1}\right) \]
\[ = |\nu_H|(-y \pm \sqrt{y^2 + 1}). \]  \hspace{1cm} (3.29)

In the last term, the \( y \)-parameter has been introduced to simplify the equation, which is defined as

\[ y = \Delta \theta(k_0 \sin 2\theta_B)/2|\nu_H|. \]  \hspace{1cm} (3.30)
\( \xi_H \) also can be obtained similarly. Considering that \( \xi_O \) is negative for \( \alpha \) branch and positive for \( \beta \) branch, we can classify all four solutions:

\[
K - K_O^\alpha = |\nu_H|(-y - \sqrt{y^2 + 1}),
\]
\[
K - K_O^\beta = |\nu_H|(-y + \sqrt{y^2 + 1}),
\]
\[
K - K_H^\alpha = |\nu_H|(y - \sqrt{y^2 + 1}),
\]
\[
K - K_H^\beta = |\nu_H|(y + \sqrt{y^2 + 1}).
\]

Using Eq. 3.21, Eq. 3.22, and Eq. 3.31 we can find unknown amplitudes \( \psi_O^{\alpha,\beta}, \psi_H^{\alpha,\beta} \):

\[
\psi_O^\alpha = \frac{1}{2}[1 - y(1 + y^2)^{-1/2}]A_0,
\]
\[
\psi_O^\beta = \frac{1}{2}[1 + y(1 + y^2)^{-1/2}]A_0,
\]
\[
\psi_H^\alpha = -\frac{1}{2}(1 + y^2)^{-1/2}\left(\frac{\nu_H}{\nu_H + \nu_H^-}\right)^{1/2}A_0,
\]
\[
\psi_H^\beta = \frac{1}{2}(1 + y^2)^{-1/2}\left(\frac{\nu_H}{\nu_H - \nu_H^-}\right)^{1/2}A_0.
\]

We can even express \( \bar{PA} \) with \( y \) and \( \theta_B \). Let’s use \( \bar{N}^{\alpha,\beta} \) for \( \bar{PA}^{\alpha,\beta} \). Then, \( \bar{N}^{\alpha,\beta} = \bar{k}_0 - \bar{K}_O^{\alpha,\beta} \) leads to

\[
\bar{N}^{\alpha,\beta} = \left\{ \frac{\nu_0}{\cos \theta_B} + \frac{|\nu_H|}{\cos \theta_B}[-y \pm (1 + y^2)^{1/2}] \right\} \hat{n},
\]

where a positive sign applies to \( \beta \) branch and a negative sign applies to \( \alpha \) branch.

### 3.1.4 Waves Leaving the Crystal

In the previous section, we have described waves inside the crystal. Once the wave leaves the crystal and travels in the free space, the wave vector must be of magnitude of \( |\bar{k}_0| \). Let \( \chi(\bar{r}) \) denote the wave function leaving the crystal. Then, from Fig. 3-3,

1. \( \angle LP = k_0 \Delta \theta \)

2. \( \angle LPM = \theta_B \)
3. $\overrightarrow{PL} = 2k_0 \Delta \theta \sin \theta_B$

4. $\overrightarrow{EH} = k_0 = k_H \therefore$ energy conservation.

Thus, we have $\vec{k}_H = \vec{k}_0 + \vec{H} - \vec{\delta}$. If we consider that $\Delta \theta$ is negative value in the figure presented here, we can rewrite $\vec{k}_H$ as

$$\vec{k}_H = \vec{k}_0 + \vec{H} + k_0 \Delta \theta \sin \theta_B \hat{n}, \quad (3.34)$$

where we define

$$\vec{\delta}(y) = k_0 \Delta \theta \sin \theta_B \hat{n}. \quad (3.35)$$

Now $\psi(\vec{r})$ inside the crystal can be expressed with $\vec{k}_0, \vec{k}_H, \vec{N}^{\alpha, \beta}$ and $\vec{\delta}$:

$$\psi(\vec{r}) = \psi_0^\alpha e^{i \vec{k}_0 \cdot \vec{r}} e^{-i \vec{N}^{\alpha, \beta} \cdot \vec{r}} + \psi_0^\beta e^{i \vec{k}_0 \cdot \vec{r}} e^{-i \vec{N}^{\alpha, \beta} \cdot \vec{r}} + \psi_H^\alpha e^{i \vec{k}_H \cdot \vec{r}} e^{-i \vec{N}^{\alpha, \beta} \cdot \vec{r}} + \psi_H^\beta e^{i \vec{k}_H \cdot \vec{r}} e^{-i \vec{N}^{\alpha, \beta} \cdot \vec{r}}. \quad (3.36)$$

Equating this with $\chi(\vec{r})$ at $\vec{r} = D \hat{n}$ where $D$ is the thickness of the crystal gives

$$\chi_0(y) = T(y) A_0 = \left[ \cos \Phi - i y (1 + y^2)^{-1/2} \sin \Phi \right] e^{i (\phi_1 - \phi_0)} A_0, \quad (3.37)$$

$$\chi_H(y) = R(y) A_0 = -i \left( \frac{\nu_H}{\nu_H^*} \right)^{1/2} (1 + y^2)^{-1/2} \sin \Phi e^{i (\phi_1 + \phi_0)} A_0,$$

where

$$\phi_0 = \nu_0 D / \cos \theta_B, \quad (3.38)$$

$$\phi_1 = y |\nu_H| D / \cos \theta_B,$$

$$\Phi = |\nu_H|(1 + y^2)^{1/2} D / \cos \theta_B.$$

Here, rapidly oscillating fringes called Pendellosung fringes can be observed from Eq. 3.37.[14]
3.2 Waves within a Perfect Crystal Interferometer

We have seen that one incident wave projected to the crystal produces four waves. Two of them are called forward rays and the other two waves are called diffracted rays. Both forward and diffracted rays have two sources they are coming from, which are $\alpha$ branch and $\beta$ branch. An LLL type interferometer has three crystal blades (Fig. 3-5). Because an incident wave splits into two spatially separated beams at the first blade, the first crystal is labelled S as in a splitter. The second crystal, M crystal, reflects some of the rays so that they can be superposed at the last analyzer crystal A. Our goal is to explain the relation between the incident angle and the directions of outgoing rays as well as the beam intensity profiles, $\Delta \theta$.

3.2.1 Current Flow inside a Crystal

As seen in Fig. 3-6 small changes in angle $\Delta \theta$ will cause enormous changes in $\Omega$ so that the wave current will span from $-\Omega$ to $+\Omega$. Thus, we can develop a general formula...
Figure 3-6: Angle amplification by small angle $\Delta \theta$.

independent of the thickness of the crystal by introducing a variable $\Gamma$ defined as

$$\Gamma = \frac{\tan \Omega}{\tan \theta_B}. \quad (3.39)$$

The angle $\Omega$ can be calculated from Fig. 3-7. From Fig. 3-7, the following relation is derived by the energy conservation law.

$$\tan \Omega (|\psi_H|^2 \cos \theta_B + |\psi_0|^2 \cos \theta_B) = |\psi_H|^2 \sin \theta_B - |\psi_0|^2 \sin \theta \quad (3.40)$$

Now we see that $\Gamma$ is a variable convenient to describe direction of rays inside a crystal. From Eq.3.32,

$$|\psi_H|^2 = \frac{1}{4} \left( \frac{1}{1 + y^2} \right) A_0^2, \quad (3.41)$$

$$|\psi_0|^2 = \frac{1}{4} \left( 1 \mp \frac{y}{\sqrt{1 + y^2}} \right)^2 A_0^2,$$
Figure 3-7: The outgoing current from one branch is the sum of forwarding and diffracted beams.

\[ \Gamma = \pm \frac{y}{\sqrt{1 + y^2}}. \]

The plus sign applies to the current from \( \alpha \) branch and the negative sign applies to the \( \beta \) branch current. Thus if we re-define

\[ \Gamma \equiv \frac{\tan \Omega^\alpha}{\tan \theta_B} = \frac{y}{(1 + y^2)^{1/2}}. \quad (3.42) \]

Then, for positive \( y \) as in Fig. 3-6, \( \alpha \) branch current goes to the positive \( \bar{H} \) direction (positive \( \Gamma \)). Similarly \( \beta \) branch current goes to the negative \( \bar{H} \) direction (negative \( \Gamma \)).

### 3.2.2 Beam Profiles between S and M Crystal

As seen in the previous section, for an incident ray from an angle \( y \), we can find four rays coming out from the crystal with thickness \( D \). They are

\[ T_\alpha = \psi_\alpha(y)e^{-iN^\alpha(y)D}, \quad (3.43) \]

\[ T_\beta = \psi_\beta(y)e^{-iN^\beta(y)D}, \]
\[ R_{\alpha} = \psi_H^\alpha(y)e^{-iN^\alpha(y)D-i\delta(y)D}, \]
\[ R_{\beta} = \psi_H^\beta(y)e^{-iN^\beta(y)D-i\delta(y)D}, \]

where \( N^{\alpha,\beta} \) is defined in Eq. 3.33 and \( \delta(y) \) is given by Eq. 3.35. Four coefficients \( \psi_O^\alpha, \psi_O^\beta, \psi_H^\alpha, \psi_H^\beta \) are also derived in Eq. 3.32. The contribution of \( \alpha \) branch current in the beam path II, between S and M crystal in Fig. 3-8, is given by

\[ I_{\alpha,r}(\Gamma) = |R_{\alpha}(y)|^2 J, \tag{3.44} \]

where \( J \) is the Jacobian that converts \( y \) coordinate to \( \Gamma \) coordinate and is defined as

\[ J = \frac{dy}{d\Gamma} = (1 - \Gamma^2)^{-3/2}. \tag{3.45} \]

For the same \( y \), \( \alpha \) branch has the exit position at \( \Gamma_S = +\Gamma \) while \( \beta \) branch current has it at \( \Gamma_S = -\Gamma \). Therefore, the total diffracted beam (or reflected beam for the subscript \( r \)) profile on path II between the first and second crystal region is

\[ I_r(\Gamma_S) = I_{\alpha,r}(\Gamma = \Gamma_S) + I_{\beta,r}(\Gamma = -\Gamma_S) \tag{3.46} \]
\[ = |R_{\alpha}(\Gamma_S)|^2 J(\Gamma_S) + |R_{\beta}(-\Gamma_S)|^2 J(-\Gamma_S) \]
\[ = \frac{1}{2}(1 - \Gamma_S^2)^{-1/2}. \]

Similarly, the forward diffracted beam profile between first and second crystal blade is given by

\[ I_f(\Gamma_S) = I_{\alpha,f}(\Gamma = \Gamma_S) + I_{\beta,f}(\Gamma = -\Gamma_S) \tag{3.47} \]
\[ = |T_{\alpha}(\Gamma_S)|^2 J(\Gamma_S) + |T_{\beta}(-\Gamma_S)|^2 J(-\Gamma_S) \]
\[ = \frac{1}{2}(1 - \Gamma_S)^2(1 - \Gamma_S^2)^{-3/2}. \]

\( I_f \) and \( I_r \) are plotted in Fig. 3-9.
Figure 3-8: Ray tracing method in an LLL type interferometer.
Figure 3-9: Averaged beam profiles between S and M crystals. $I_t$ diverges at $\Gamma = -1$ and $I_r$ diverges at both edges.

\[ I_t(\Gamma) = \left( \frac{1}{2} \right) (1-\Gamma^2) \left( 1-\Gamma^2 \right)^{-3/2} \]

\[ I_r(\Gamma) = \left( \frac{1}{2} \right) (1-\Gamma^2)^{-1/2} \]
3.2.3 Spatial Profiles of the Interfering Beam

Just as we have done in the previous section, we can trace all interfering rays from Fig. 3-8. O beam and H beam, each consists of four rays coming from points \( a, b, c, d \). And these four rays are four results of six rays in the region between M and A crystals. Let’s define rays from the left in Fig. 3-8:

\[
\begin{align*}
\Lambda_1 &= R_\alpha(y)R_\alpha(-y)e^{-i\Delta\beta}, \\
\Lambda_2 &= (R_\alpha(y)R_\beta(-Y) + R_\beta(y)R_\alpha(-y))e^{-i\Delta\beta}, \\
\Lambda_3 &= R_\beta(y)R_\beta(-y)e^{-i\Delta\beta}, \\
\Lambda_4 &= T_\alpha(y)R_\alpha(y), \\
\Lambda_5 &= T_\alpha(y)R_\beta(y) + T_\beta(y)R_\alpha(y), \\
\Lambda_6 &= T_\beta(y)R_\beta(y).
\end{align*}
\]

Then, amplitudes for each four rays for both O beam and H beam is given by

\[
\begin{align*}
\chi_{O,a} &= \Lambda_1 T_\alpha(y) + \Lambda_4 R_\alpha(-y), \\
\chi_{O,b} &= \Lambda_1 T_\beta(y) + \Lambda_2 T_\alpha(y) + \Lambda_4 R_\beta(-y) + \Lambda_5 R_\alpha(-y), \\
\chi_{O,c} &= \Lambda_2 T_\beta(y) + \Lambda_3 T_\alpha(y) + \Lambda_5 R_\beta(-y) + \Lambda_6 R_\alpha(-y), \\
\chi_{O,d} &= \Lambda_3 T_\beta(y) + \Lambda_6 R_\beta(-y), \\
\chi_{H,a} &= \Lambda_1 R_\alpha(y) + \Lambda_4 T_\alpha(-y), \\
\chi_{H,b} &= \Lambda_1 R_\beta(y) + \Lambda_2 R_\alpha(y) + \Lambda_4 T_\beta(-y) + \Lambda_5 T_\alpha(-y), \\
\chi_{H,c} &= \Lambda_2 R_\beta(y) + \Lambda_3 R_\alpha(y) + \Lambda_5 T_\beta(-y) + \Lambda_6 T_\alpha(-y), \\
\chi_{H,d} &= \Lambda_3 R_\beta(y) + \Lambda_6 T_\beta(-y).
\end{align*}
\]

Now, one can calculate intensities of each ray by substituting \( \Lambda \) into Eq. 3.49 Then,

\[
I_{O,a}(\Gamma) = I_{O,d}(\Gamma) = \frac{1}{32}(1 - \Gamma)^2(1 - \Gamma^2)^{1/2}(1 + \cos\Delta\beta),
\]

(3.50)
Figure 3-10: Intensity profiles. The number of neutrons arriving at detectors can be obtained by calculating the area under the intensity curves.

\[
I_{O,b}(\Gamma) = \frac{1}{32}(1 - \Gamma^2)^{1/2}(3\Gamma - 1)^2(1 + \cos \Delta \beta),
\]
\[
I_{O,c}(\Gamma) = \frac{1}{32}(1 - \Gamma^2)^{1/2}(3\Gamma + 1)^2(1 + \cos \Delta \beta),
\]
\[
I_{H,a}(\Gamma) = I_{H,d}(\Gamma) = \frac{1}{32}(1 - \Gamma^2)^{3/2}(1 + \cos \Delta \beta),
\]
\[
I_{H,b}(\Gamma) = I_{H,c}(\Gamma) = \frac{1}{64}[9(1 - \Gamma^2)^{3/2} + (3\Gamma^2 + 1)^2(1 - \Gamma^2)^{-1/2} - 6(3\Gamma^2 + 1)(1 - \Gamma^2)^{1/2}\cos \Delta \beta].
\]

Here, one has to note that \(I_{O,a}, I_{O,d}, I_{H,a}, I_{H,d}\) are valid for \(-3 \leq \Gamma_A \leq +3\), while other functions are valid only for \(-1 \leq \Gamma_A \leq +1\). As a result, the intensity profiles after the last blade of a perfect crystal look like Fig. 3-10. The average number of neutrons arriving at the detectors can be calculated by integrating Eq. 3.51 over \(\Gamma\). Since we are not interested in spatial distribution of intensities, integration can be performed without the Jacobian.
As a result, we find

\[ I_O(\Gamma, \Delta \beta) = a_O(\Gamma) + b_O(\Gamma) \cos \Delta \beta, \]  
\[ I_H(\Gamma, \Delta \beta) = a_H(\Gamma) + b_H(\Gamma) \cos \Delta \beta. \]  

with coefficients,

\[ a_O(\Gamma) = \frac{1}{8}(1 - \Gamma^2)^{1/2}(1 + 5 \Gamma^2), \]  
\[ a_H(\Gamma) = \frac{1}{8}(1 - \Gamma^2)^{-1/2}(5 \Gamma^4 - 4 \Gamma^2 + 3), \]  
\[ b_O(\Gamma) = \frac{1}{8}(1 - \Gamma^2)^{1/2}(1 + 5 \Gamma^2), \]  
\[ b_H(\Gamma) = -\frac{1}{8}(1 - \Gamma^2)^{1/2}(1 + 5 \Gamma^2). \]

Now we integrate over \( \Gamma \) and obtain:

\[ I_O(\Delta \beta) = \int_{-1}^{1} I_O(\Gamma, \Delta \beta) d\Gamma \]  
\[ = \int_{-1}^{1} a_O(\Gamma) d\Gamma + \int_{-1}^{1} b_O(\Gamma) d\Gamma \cdot \cos \Delta \beta \]  
\[ = \frac{9\pi}{64}(1 + \cos \Delta \beta), \]  
\[ I_H(\Delta \beta) = \int_{-1}^{1} a_H(\Gamma) d\Gamma + \int_{-1}^{1} b_H(\Gamma) d\Gamma \cdot \cos \Delta \beta \]  
\[ = \frac{23\pi}{64} - \frac{9\pi}{64} \cos \Delta \beta \]

In many cases, the contrast turns out to be useful in experiment. From the above result, it is apparent that the O beam has 100 percent contrast while the H beam has 39.1 percent contrast. In principle the detector should be very wide to count all neutrons coming from the last crystal blade. If the detector fails to capture all neutrons, the intensity predicted here may fail and change the contrast too. It is also interesting to see that the contrast has a spatial profile for H beam (Fig. 3-11). Since
spatial distribution interests us, $\Gamma_A$ has to be taken into account carefully. If we write

$$I_H(\Gamma_A) = I_H^0(\Gamma_A) + I_H^1(\Gamma_A) + I_H^2(\Gamma_A) + I_H^3(\Gamma_A)$$

$$= a_H'(\Gamma_A) + b_H(\Gamma_A) \cos \Delta \beta, \quad |\Gamma_A| \leq 1$$

$$= a_H''(\Gamma_A) + b_H'(\Gamma_A) \cos \Delta \beta, \quad |\Gamma_A| \geq 1,$$  \hspace{1cm} (3.54)

the contrast of H beam is 100 percent for $|\Gamma_A| \geq 1$, while the contrast for $|\Gamma_A| \leq 1$ is given by

$$C(\Gamma) = \frac{(a_H'(\Gamma) - b_H'(\Gamma)) - (a_H'(\Gamma) + b_H'(\Gamma))}{(a_H'(\Gamma) - b_H'(\Gamma)) + (a_H'(\Gamma) + b_H'(\Gamma))}$$

$$= \frac{-2b_H'(\Gamma)}{2a_H'(\Gamma)}$$

$$= \frac{(2/64)(6\Gamma_A^2 + 1)(1 - \Gamma_A^2)^{1/2} - (2/96)(1 - (\Gamma_A/3)^2)^{3/2}}{(2/96)(1 - (\Gamma_A/3)^2)^{3/2} + (2/64)(9(1 - \Gamma_A^2)^{3/2} + (3\Gamma_A^2 + 1)^2(1 - \Gamma_A^2)^{-1/2})}$$
Figure 3-11: The contrast profile of an H beam. In theory, the contrast of an O beam is 100 percent.
Chapter 4

Experiment

We use the fact that neutron waves accumulate phases when neutrons pass through low absorbing materials. The phase is directly related to the scattering cross section of the material used. Spatial encoding of the phase is made possible by use of aluminium wedges.

4.1 Apparatus

4.1.1 Interferometer

A perfect crystal with three blades, an LLL type interferometer, was used and the experiment was done at Neutron Interferometry Facility at National Institute of Standards and Technology (NIST) with the collaboration of the neutron interferometry group led by Dr. Arif.

As seen from Fig. 4-1 the perfect crystal is located at a specially designed chamber where most vibrations are isolated by the state-of-the-art pressure control table.

4.1.2 Wedge

The material used to make wedges and samples is called 6061 Al. This Aluminium alloy has good formability and corrosion resistance with medium strength. Compositions of 6061 Al are shown in Table 4.1. From the composition table, it can be
Figure 4-1: A sketch of reciprocal space neutron imaging. The second monochrometer is a focusing monochrometer.
<table>
<thead>
<tr>
<th>Material</th>
<th>Ratio(%) by atoms</th>
<th>( N(\times10^{22} \text{ atoms/cm}^3) )</th>
<th>( b_\text{c} ) (fm)</th>
<th>( Nb_\text{c}(\text{atoms/cm}^2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>0.581</td>
<td>4.994</td>
<td>4.15</td>
<td>( 1.204 \times 10^8 )</td>
</tr>
<tr>
<td>Fe</td>
<td>0.341</td>
<td>8.488</td>
<td>9.45</td>
<td>( 2.735 \times 10^8 )</td>
</tr>
<tr>
<td>Cu</td>
<td>0.118</td>
<td>8.488</td>
<td>7.718</td>
<td>( 7.730 \times 10^7 )</td>
</tr>
<tr>
<td>Mn</td>
<td>0.074</td>
<td>7.901</td>
<td>-3.75</td>
<td>( -2.193 \times 10^7 )</td>
</tr>
<tr>
<td>Mg</td>
<td>1.187</td>
<td>4.305</td>
<td>5.375</td>
<td>( 2.754 \times 10^7 )</td>
</tr>
<tr>
<td>Cr</td>
<td>0.102</td>
<td>8.315</td>
<td>3.635</td>
<td>( 3.083 \times 10^7 )</td>
</tr>
<tr>
<td>Zn</td>
<td>0.104</td>
<td>6.567</td>
<td>5.680</td>
<td>( 3.879 \times 10^7 )</td>
</tr>
<tr>
<td>Ti</td>
<td>0.085</td>
<td>5.709</td>
<td>-3.459</td>
<td>( -1.668 \times 10^7 )</td>
</tr>
<tr>
<td>Al</td>
<td>97.475</td>
<td>6.022</td>
<td>3.449</td>
<td>( 2.02454 \times 10^{10} )</td>
</tr>
</tbody>
</table>

Table 4.1: 6061 Aluminium alloy composition

calculated that \( 2\pi \) phase change requires that a neutron should travel 111.4 \( \mu \)m of 6061 Al material for 2.71 Å wavelength beam. The path length required for wavelength \( \lambda \) to have \( 2\pi \) phase change is plotted in Fig. 4-2. There are two methods used to make phase gradients. A single wedge (Fig. 4-3) is designed to produce different phase gradients by rotating it around the beam path axis. Since the width of the neutron beam cannot be ignored for the beam between S and M crystal (Fig. 4-4), the gradient along y direction naturally appears, which makes a more complicated phase distribution than the other wedge type, a wedge assembly.

A wedge assembly is designed to create one directional gradients only. As in Fig. 4-5 there are 10 small non-zero gradient wedges on each wheel. Each wedge is 10 mm × 4 mm size. On the back of each wheel, we attached a Cd mask to constrain the beam more precisely. A Cd mask has 12 holes of 3 mm × 8 mm size including zero gradient position.

### 4.1.3 Wedge Control

A single wedge or wedge assembly should be attached to a wedge holder. Wedges are rotated around the beam axis by the small rotation motor attached to this wedge holder (Fig. 4-4). As a result, a single wedge acquires various phase gradients and a wedge assembly can change the wheel section to get a different set of gradients into the beam path.
Figure 4-2: The circle on the line indicates that $2\pi$ phase change is made when the path length of a neutron through the 6061 Al material is 111.449 $\mu$m.
Figure 4-3: A single wedge is rotating around the beam axis ($x$ axis). The phase distribution is plotted as $\cos \phi(y, z)$ near single wedges.
Figure 4-4: A Single wedge is held by a wedge holder. The rotation motor attached to the wedge holder rotates the single wedge around beam axis.
Figure 4-5: There are 48 phase gradients. Each gradient is a small version of a single wedge.
4.1.4 Mount

Since the crystal is too fragile, everything has to be held from the top or side and carefully controlled by motors. A wedge holder is held from the top and is attached to a translational motor to move parallel to the crystal blade. There are two uses for this translational motor. One is to calibrate beam position to make sure if the wedge is placed in the right beam path. The other is to select different gradients of a wedge assembly.

4.1.5 Sample

The sample is designed to produce no more than a $2\pi/4$ phase change. The sample has a height of 15 mm and 10 mm width. The phase shift $\chi$ for a beam traversing a medium is complex and is given by

$$\chi = k(1 - n)D_{eff} = \chi' + i\chi''$$

(4.1)

where $D_{eff}$ is the effective path length of the beam in the material medium, $n$ is the index of refraction of the material and $k$ is the wave vector of the neutron beam. $\chi''$ usually reduces the intensity but does nothing to the phase of the neutron. For thermal neutrons, in which the energy is much larger than the mean interaction potential and low-absorbing materials, the index of refraction and the phase shift simplify to

$$n = 1 - \lambda^2 \frac{N b_c}{2\pi} \quad \text{and} \quad \chi' = -N b_c \lambda D.$$  

(4.2)

Here, $N$ is a particle density and $b_c$ is the mean coherent scattering length with $\lambda$ as a wavelength of the neutron beam. We are focusing on a sample which will result in the maximum phase difference of $2\pi$. In other words $N b_c \lambda D < 2\pi$ is the range we are looking in the sample material. The dimension I have chosen for sample is shown in Fig. 4-6.
Figure 4-6: The dimension of sample is chosen so that the phase difference of $\phi \leq 2\pi/4$ can be observed.
4.2 Measurement Process

4.2.1 Single Wedge

Once we locate the beam position (or beam trajectory), the wedge holder is properly positioned so that the neutron beam can pass through the simple wedge as in Fig. 4-4. Starting from maximum $z$ direction gradient, when the wedge rotation angle is zero, the counting continues for every step angle until the wedge is rotated by $90^\circ$. After one measurement of 12 minutes long is completed, the wedge rotator equipped with the wedge holder rotates the single wedge around the beam axis for one step degree. As a result, neutron beam acquires a new phase profile. The measurement went on from $-10^\circ$ to $100^\circ$ of the beam axis rotator motion. After one cycle of measurement is done, the imaging sample piece is inserted in the beam path I, and the same measurement is performed (Fig. 4-4).

4.2.2 Wedge Assembly: Calibration

Unlike the single wedge, a wedge assembly is consist of many wedges with different gradients. Even though each wedge constituting a wedge assembly is well crafted by diamond drill machining, it is safe to consider possible variations of the base thicknesses of wedges. If we express the base thickness as $g_0$, the spatial phase distribution along $z$ direction can be written as

$$\Delta \beta(z) = k_i z + g_{0,i}, \quad (4.3)$$

where $k_i$ is the gradient of $i$th wedge and $g_{0,i}$ is the base thickness of it. Then, the intensity profile reads

$$I_0(k_i) = \int z \left( a_O + b_O \cos(k_i z + g_{0,i} + \phi(z)) \right) dz \quad (4.4)$$

with an unknown profile of a sample, $\phi(z)$. It is the rate of change of phase that makes it possible to do Fourier analysis in reciprocal space imaging. Thus, we don’t want
obtain encoded phase profile over the wedge. In Fig. 4-8, the thickness profile of the wedge including the base thickness is plotted with one example of phase contrast scans.

For the calibration process, we select one $Z_0$ as the reference point, and define the origin of $z$ coordinate as $Z_0$. From the phase contrast scan, maximum intensity peaks (Fig. 4-8) can be found for each wedge of a wedge assembly, and each peak
Figure 4-8: Phase profile of a wedge measured along the z direction is plotted. The gradient is calculated to be $356^\circ/mm$, which is very close to $2\pi$ rad/mm. One example of phase contrast scans is shown with contrast of 14 percent.
indicates the phase shifter angle that the phase accumulated at point \( Z_0 \) is an integer multiple of \( 2\pi \). Thus, the phase shifter rotation angle values are recorded and used as reference points in main imaging measurements.

### 4.2.3 Wedge Assembly: K-space scan

As one can see from Fig. 4-5, small wedges that fit the beam size are aligned on each wheel. There are 48 gradient wedges carved on the wedge assembly plate. Twenty of them are phase gradients from \( 2\pi/20 \) rad/mm to \( 2\pi \) rad/mm, and they are the wedges aligned along the outer side of the wheels. Another 20 small wedges produce phase gradients from \( -2\pi/20 \) rad/mm to \( -2\pi \) rad/mm that are located along the inner side of the wheels. And there are 8 zero gradients, two on each wheel.

The first measurement starts from the zero gradient wedge on the outer side of the wheel. After one hour of counting, the wedge holder is translated to the next gradient position by the translation motor on the top cover glass (Fig. 4-9). The outer gradient scan is completed after six measurements. Then, the wedge holder moves down, driven by the vertical translation motor (Fig. 4-9) which is also on the top cover. Measurements with negative gradients is performed with inner an wedge set just like the measurements with an outer wedge set before. Once 12 measurements are taken with one section of the wheel, the wedge rotator rotates the wedge assembly 90 degrees around the beam axis so that another set of gradients can be used for phase encoding. After 48 wedge scans are completed, the imaging sample is inserted in beam path I for another cycle of measurement.

### 4.3 Theoretical Prediction

With the help of the dynamical diffraction theory discussed in previous chapters, I have performed forwarding simulations of the experiment described above.
Figure 4-9: Wedge assembly is translated horizontally or vertically to select a proper phase gradient.

### 4.3.1 Single Wedge

Eq. 4.2 can be applied to the neutron phase picked up through the wedge. Then, the phase term from Eq. 3.50 may be written as

\[ e^{-i\Delta \beta} = e^{-i\chi'} = e^{iN\beta_c \lambda D}. \tag{4.5} \]

Since \( N, \beta_c, \lambda \) are constants representing a number density, bound coherence scattering length and wavelength of the neutron beam, what determines the spatial phase profile of the neutron beam passing through the wedge is the geometry of the wedge, \( D(z) \). We use a single wedge with specific \( D(z) \) so that the resulting variable \( N\beta_c \lambda D(z) \) can be rewritten as \( kz \) where \( k \) is the magnitude of the gradient and \( z \) is the vertical coordinate. For the experiment, \( D(z) \) is chosen in a way that the gradient \( k \) is equal to \( 2\pi \text{ rad/mm} \). But since we are rotating the simple wedge around the beam axis the phase profile \( \chi' \) depends on the \( y \) axis too (Fig. 4-3). Then, \( k \) is given as a function of the rotation angle

\[ k(\theta) = k \cos \theta \hat{z} + k \sin \theta \hat{y}. \tag{4.6} \]
Therefore,

\[ \Delta \beta = k z \cos \theta + ky \sin \theta + \delta_{sw}, \]  

(4.7)

\[ I_O(\Gamma, \theta) = a_O(\Gamma)[1 + \cos(kz \cos \theta + ky \sin \theta + \delta_{sw})], \]

\[ I_H(\Gamma, \theta) = a_H(\Gamma) + b_H(\Gamma) \cos(kz \cos \theta + ky \sin \theta + \delta_{sw}), \]

(4.8)

where \( \delta_{sw} \) is the phase from the overall constant thickness. For the neutron beam size of \( 2w \times 2h \) mm (width \times height), \( y = w \Gamma \) is valid. Then,

\[ I_O(\theta) = \int_{\Gamma=-1}^{1} \int_{z=-h}^{h} a_O(\Gamma)[1 + \cos(kz \cos \theta + kw \Gamma \sin \theta)] d\Gamma dz, \]

(4.8)

\[ I_H(\theta) = \int_{\Gamma=-1}^{1} \int_{z=-h}^{h} a_H(\Gamma) + b_H(\Gamma) \cos(kz \cos \theta + kw \Gamma \sin \theta) d\Gamma dz. \]

With \( h = 4 \) mm, \( w = 1.5 \) mm, \( I_O \) and \( I_H \) are plotted in Fig. 4-10. The result with the sample profile of \( \phi(z) \) is also plotted in the same figure. Here, the sample has been generated according to the design given in Fig. 4-6.

### 4.3.2 Wedge Assembly Simulation

The wedge assembly has a set of wedges with the \( z \)-directional phase gradient. Therefore,

\[ \Delta \beta = k_i z \]

(4.9)

where \( i \) is the index of gradients that the \( i \)th wedge has. Then,

\[ I_O = \int_{\Gamma=-1}^{1} \int_{z=-h}^{h} a_O(\Gamma) + b_O(\Gamma) \cos(k_i z + \delta_{wa} + \phi(z)) d\Gamma dz, \]

(4.10)

\[ I_H = \int_{\gamma=-1}^{1} \int_{z=-h}^{h} a_H(\Gamma) + b_H(\Gamma) \cos(k_i z + \delta_{wa} + \phi(z)) d\Gamma dz. \]

The simulation result without a sample is plotted for the O-beam case in Fig. 4-11. The result with the sample phase profile \( \phi(z) \) is in Fig. 4-12. In Fig. 4-11, the Fourier transform of a beam profile, when the beam slit is 8 mm high, is shown in a dashed line. The \( x \) axis range of a dashed line indicates the maximum resolution that can
Figure 4-10: Simulation results of a single wedge experiment. The result with a sample in beam path I is also plotted.
Figure 4-11: Simulation results of wedge assembly experiment. Since wedge assembly consists of both positive and negative gradients, the simulation is also performed with both gradients. Fourier transform of beam profile with an 8 mm high slit is shown with a dashed line.
Figure 4-12: Wedge assembly experiment with a sample in beam path I. The dashed line indicates the beam profile convoluted with the sample profile in Fourier space.
be achieved with the gradient considered here. Overall amplitude decreases as the gradient increases. Therefore, we expect to see less contrast with a higher gradient. The ratio of the O-beam intensity to the Fourier transform of a beam profile can be interpreted as a modulation transfer function. But when there is a sample in the beam path, the O-beam intensity is not simply $MTF \times FT[Beam(z) \otimes Sample(z)]$, which is generally true for Fourier imaging. This is because the interferogram cannot be written in an exact Fourier form (Eq. 4.10). Thus an algorithm different from the inverse Fourier transform has to be introduced to reconstruct the image from acquired experimental data.

## 4.4 Experiment Result

### 4.4.1 Single Wedge

The results are plotted in Fig. 4-13 and Fig. 4-14. The wedge rotates from 0 to 90° around the beam axis. Every 1° rotation, neutrons are counted for 720 seconds without a sample and 30 minutes with a sample. Then, data are normalized to produce constant incoming neutron monitor counts. The contrast is relatively low, 5 percent for both experiments. There are apparent discrepancies between the data with a sample in the beam path and the data without a sample, which indicates that the scattering cross section profile of the sample affects the phase distribution of the neutron beam. But due to the low contrast, it is almost impossible to reconstruct the sample’s image. In Fig. 4-15, the simulation result from Eq. 4.8 is shown with the experiment data for the case when the sample is out of the beam path. The raw data has been normalized properly to visualize the magnitude of discrepancy. The disagreement between the model (Eq. 4.8) and the experiment data suggests that the model needs improvement. Therefore, we have implemented intrinsic thickness to the single wedge, which is expressed as a constant phase term $\phi_0$. A possible orientation error in rotation angles is also considered by adding $\theta_0$ variable into $\sin \theta$ and $\cos \theta$. Another consideration comes from the fact that the beam size between the S and M
Figure 4-13: The result from single wedge experiment plotted. A sample is not considered in this case.
Figure 4-14: The single wedge experiment result with a sample in the beam path.
Figure 4-15: Simulation results are plotted with the raw data of O-beam normalized arbitrarily.
crystals may not be the size we predict from the geometry of the crystal. Therefore, four more variables are added, which will limit the boundaries of integration in Eq. 4.8. If we add these variables to the interference model, we have a following relation:

$$I(\theta) = I_0 \int_{y_i}^{y_f} \int_{z_i}^{z_f} |e^{ikz \cos(\theta - \theta_0)} e^{iky \sin(\theta - \theta_0)} + e^{i\phi_0}|^2 dydz$$

(4.11)

$I(\theta)$ is now a function of $I_0, k, \phi_0, \theta, \theta_0, x_f, x_i, z_f, z_i$, where $k$ is also considered to be a variable. Using a least square method, a better fitting curve can be obtained (Fig. 4-16). It has to be noted that $k$ is close to $2\pi$, and the beam size obtained from the fitting is also close to the geometric prediction $3$ mm $\times$ $8$ mm (width $\times$ height).

4.4.2 Wedge Assembly

There were 41 measurements involved for one scan. The gradient varies from $-2\pi$ rad/mm to $+2\pi$ rad/mm at a constant step size. The results are shown in Fig. 4-17 and Fig. 4-18 with the curve predicted by the dynamical diffraction theory. The detector were turned on for about an hour for each measurement point. The average contrast is about 10 percent, which is a little larger than the contrast in a single wedge experiment. Since we have comparably uniform y-directional phase changes with a wedge assembly, the integration involved in the intensity calculation is performed in a constructive way. As a result, a higher average contrast is achieved. But there are still large discrepancies between raw data and the predicted lines. The major contrast loss can be explained by the beam intensity distribution between S and M crystals. Most of the intensity was concentrated at one side of the beam as seen from Fig. 3-9. Therefore, the effort to separate each wedge from another by covering it with a Cd mask caused major intensity loss rather than providing a uniform and discrete gradient.
Figure 4-16: Fitting with an improved model. Variables were found to be $k = 6.29$, $\phi_0 = 4.92$, $\theta_0 = 0.15$, $x_i = -2.47$, $x_f = 1.39$, $z_i = -4.53$, $z_f = 3.08$. 
Figure 4-17: For the high gradient region, the graph shows oscillations similar to ones from the beam profile.
Figure 4-18: Discrepancies turned out to be too large for imaging reconstruction.
Chapter 5

Conclusion

We showed a newly proposed reciprocal space neutron imaging method. Combined with a perfect crystal and with phase gradient wedges, we were able to encode spatially distributed phase information. With a single wedge experiment, we have discovered a new way of beam profiling without a position-sensitive detector. A wedge assembly experiment provides a good starting point of reciprocal space neutron imaging by showing that the spatial phase encoding is indeed possible (Fig. 5-1).

There are several problems that have to be solved before the reciprocal space neutron imaging can be applied as an alternative imaging method of real space imaging. First, the gradient has to be made with fewer errors. In our experiment, even small errors less than 0.1 mm could cause $2\pi$ phase change of a neutron. Second, to make use of as many neutrons as possible, the gradient has to cover a complete beam width, and horizontal homogeneity of the gradient is a crucial factor for a high contrast. In other words, the phase distribution encoded by the wedge has to be given as a function of $z$, i.e. $kz$, and should not depend on other coordinate variables. One way to solve these problems is to make a phase gradient using a magnetic field. A gradient coil pair can be designed by combining two circular current loops with opposite current directions. The gradient field generated around the coil is described in Fig. 5-2. Then, instead of using a scattering cross-sectional phase of a neutron, we use spin phase degrees of freedom to encode phase gradient as in Fig. 5-3.

In Fig. 5-3, polarized incident neutrons enter the gradient coil. Then, a spin phase
Figure 5-1: The O beam is observed with a position-sensitive detector when a gradient wedge is in the beam path. The periodic interferogram shows that the phase is indeed encoded spatially according to the value of the gradient of the wedge.
Figure 5-2: The gradient field produced by a gradient coil pair. $B_z$ is drawn around the center of the coils. The inhomogeneity is the key to create a spin phase gradient.

Figure 5-3: Sketch of magnetic gradient reciprocal space neutron imaging. To make use of a spin degree of freedom, the neutron beam has to be polarized before entering the crystal.
gradient is formed due to the inhomogeneous spatial distribution of the magnetic field produced by the gradient coil pair. The current controlled magnetic gradient will provide much more flexibility in control of magnitudes of gradients. Therefore, using a magnetic field gradient coil pair, we expect to develop a reciprocal space neutron imaging method as an alternative method of real space imaging.
Bibliography


