Principles of X-ray Crystallography

Advisor: Raymond Kwok, Ph.D.
Coadvisor: Sotoudeh Hamedi-Hagh, Ph.D.
Committee Member: Masoud Mostafavi, Ph.D.
Supervisor: Tri Caohuu, Ph.D.

Luke Snow
58 Mount Hermon Rd
Scotts Valley, CA 95066
(831) 440-9170
LukeSnow@Gmail.com
Abstract

• The goal of this paper is to verify the principles of crystallography at radio-frequencies, and then use the principles to design an antenna.
Outline

• Motivation and Introduction
• Verify Principles
  – Bragg’s Law
  – Scherrer Law
• Experimental Verification
• Switched beam design
• Conclusion and Further Work
The Classic Experimental Setup

- X-ray source
- Incident Beam
- Sample
- Diffracted Beam
- Detector
- $2\theta$
Some Typical Data...
Some Typical Data…
Principles of X-ray Diffraction

• Bragg’s Law
• The Scherrer Equation
• The Reciprocal Lattice
• The Ewald Sphere
• The Scattering Factor
Motivation and Methodology

- To apply the concepts verified to design an antenna.
- To verify the concepts, the flow chart at right was used.
Motivation and Methodology

• The concepts verified were employed to design an antenna, shown in the flow chart.
Background

- X-ray Crystallography is a well established field.
- Born with the Discovery of Bragg’s Law, in 1912.
- Basic principles are used to determine crystal structure, size, and defects.
Photonic Crystals

- Pioneered by E. Yablonovitch in 1987.
- Most applications employ the band stop and band pass properties of photonic crystals
  - Beam focusing antenna substrate
  - Tunable 4-port switch
  - Band pass or band block filters
Antenna

• The design can be thought of as an antenna array.
• The design presented, and the analysis behind it, appear to be unique.
Direction of Main Lobe

- The direction of the main lobe of the antenna is determined by Bragg’s Law:
  \[ \lambda = 2d \sin \theta \]
Sample Level View

k → Crystal → k'

θ → 2θ → 0
Bragg’s Law Verified
Experimental Setup

Top View

Skewed View
Results
## Summary – Peak Locations

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<thead>
<tr>
<th>Predicted</th>
<th>Observed</th>
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<td>22</td>
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<tr>
<td>24</td>
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<tr>
<td>26</td>
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<td>46</td>
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<td>Avg:</td>
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<tr>
<td>RSD</td>
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Beam Width

- The beam width (FWHM) is given by the Scherrer Law:
  \[ B(2\theta) = \frac{K\lambda}{(Na \cos \theta)} \]
- K - shape factor
- N - size of the crystal in unit cells
- a - unit cell length for a square crystal
- \( \lambda \) - Wavelength
- \( \theta \) - Bragg angle
Verification

• The Scherrer law is verified in two ways
  – By varying N, holding all other quantities constant. Expect a 1/N dependence, and values of K on the order of unity.
  – Vary $\theta$ and a together; Use Bragg’s Law to substitute for $a$ in the Scherrer equation:
    $B(2\theta) = 2K \tan \theta / N$
Results

K = 1.02 Gave Best Fit
Results

Effect of Angle On Peak Width

K = 0.90 Gave Best Fit
Experimental

• An antenna was constructed to verify Bragg’s law.
• The antenna consisted of a waveguide, horn, and a parallel plate/crystal section.
• The antenna was designed to operate in the 6GHz region.
Experimental

• Data was taken in a Compact Antenna Test Range (CATR).
• A VNA with 0-40GHz capability was used to take data.
• A WR137 waveguide to coax adapter was used for the detector.
• Two WR137 waveguides were used for a reference.
• Far Field for this design was 12 ft.
• Data was taken at approximately 14ft, for an angular resolution of 0.5 deg.
## Waveguide section

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<td>ID</td>
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<td>$f_{c10}$</td>
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<td>$f_{c11}$</td>
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Horn Section

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<td>$a$</td>
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<td>$\rho_1$</td>
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Parallel Plate Section

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<td>d</td>
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<td>$f_{c00}$</td>
<td>0 GHz</td>
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<tr>
<td>$f_{c10}$</td>
<td>6 GHz</td>
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<tr>
<td>Post Diam</td>
<td>1/8&quot;</td>
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<tr>
<td>-----------</td>
<td>------</td>
</tr>
<tr>
<td>θ</td>
<td>30°</td>
</tr>
<tr>
<td>λ</td>
<td>2&quot;</td>
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Crystal Section

![Crystal Section Diagram]

- Post Diam: 1/8"
- θ: 30°
- λ: 2"
- 12 in x 12 in
- 30deg
- 1 in
- 2 in
- 12 in
Results

• Return Loss was better than –20dB at 5.9GHz, and was about –10dB at 6.223GHz
• 5.9GHz corresponds to a wavelength of 2in, but the best performance was obtained at 6.223GHz, with a gain over WR137 of 8dB
Results

Transmission, 5.9GHz

HFSS Data, 6GHz
The best radiation pattern obtained

30 degree incidence
A polar plot
Results

Transmission, 6.223 GHz
Frequency of Max transmission at 150 deg.

Best Performance
Conclusions and Observations

• Design could be improved with:
  – Better grounding
  – Higher quality plane wave.
  – Larger diameter posts
  – Longer interaction length
Switched Beam Antenna

- Each Crystal has an associated “reciprocal space” – a lattice of points related to those of the direct space crystal.
- The units of this space are inverse length.
- For a direct space rectangular lattice of dimensions a and b, the reciprocal lattice is of rectangular, of length $\frac{1}{a}$, $\frac{1}{b}$.
- The “Ewald Circle” may be drawn in reciprocal space to describe an X-ray diffraction experiment, the circle having radius $\frac{1}{\lambda}$
- When the circle intersects two or more reciprocal lattice points, one or more reflections are created.
For the given diagram, there are two 45 degree reflections. If $a = b = 0.5\text{in}$, then $\lambda = 0.707\text{in}$
The reciprocal lattice has been altered by doubling the length of the basis vector in the vertical direction, corresponding to halving the direct-space lattice basis vector.
The two models
The two radiation patterns

RectCryst2Lobes

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<tr>
<td>m3</td>
<td>126.0000</td>
<td>0.7572</td>
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RectCryst1Lobe

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<td>m2</td>
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Conclusion

• Various concepts of crystallography have been verified.
• Fruitful parallels between X-ray diffraction and photonic crystals exist, with potential to illuminate ideas in both fields.
• More work to be done before the design is admitted to practical application.
  – Additional Measurements with the improved model
  – Switched beam measurement
Pattern after Improvement
References

- Data Taken in Upper Division Physics Lab, University of California, Santa Cruz, 2001
Acknowledgements

- My advisor, Dr. Ray Kwok
- Bill Shull of Zygo corporation, for helping with the construction of the antenna, and use of his Machine Shop,
- My Supervisor and co-workers at Space Systems Loral, for providing facilities and assistance to make the measurements.
- My Wife and family, for their patience with my seemingly endless project.
Questions?
The effect of Post Diameter

Effect of Post Size

- Diffracted Beam Peak
- Straight Through Beam

Intensity of Peak (mV) vs. Post Diameter (cm)
# Model Specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Plate Thickness - Top</td>
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<tr>
<td>Plate Thickness - Bottom</td>
<td>0.1cm</td>
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<tr>
<td>Plate Spacing</td>
<td>1.25cm</td>
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<tr>
<td>Crystal Size</td>
<td>8x8</td>
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<tr>
<td>Post Spacing</td>
<td>$\lambda/(2 \sin \theta)$</td>
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<tr>
<td>Post Radius</td>
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<tr>
<td>Angle of Incidence</td>
<td>$22^\circ$-$46^\circ$, $2^\circ$ steps; $45^\circ$</td>
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<tr>
<td>Solution Frequency</td>
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<td>Max. $\Delta S$</td>
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