Principles of X-ray Crystallography

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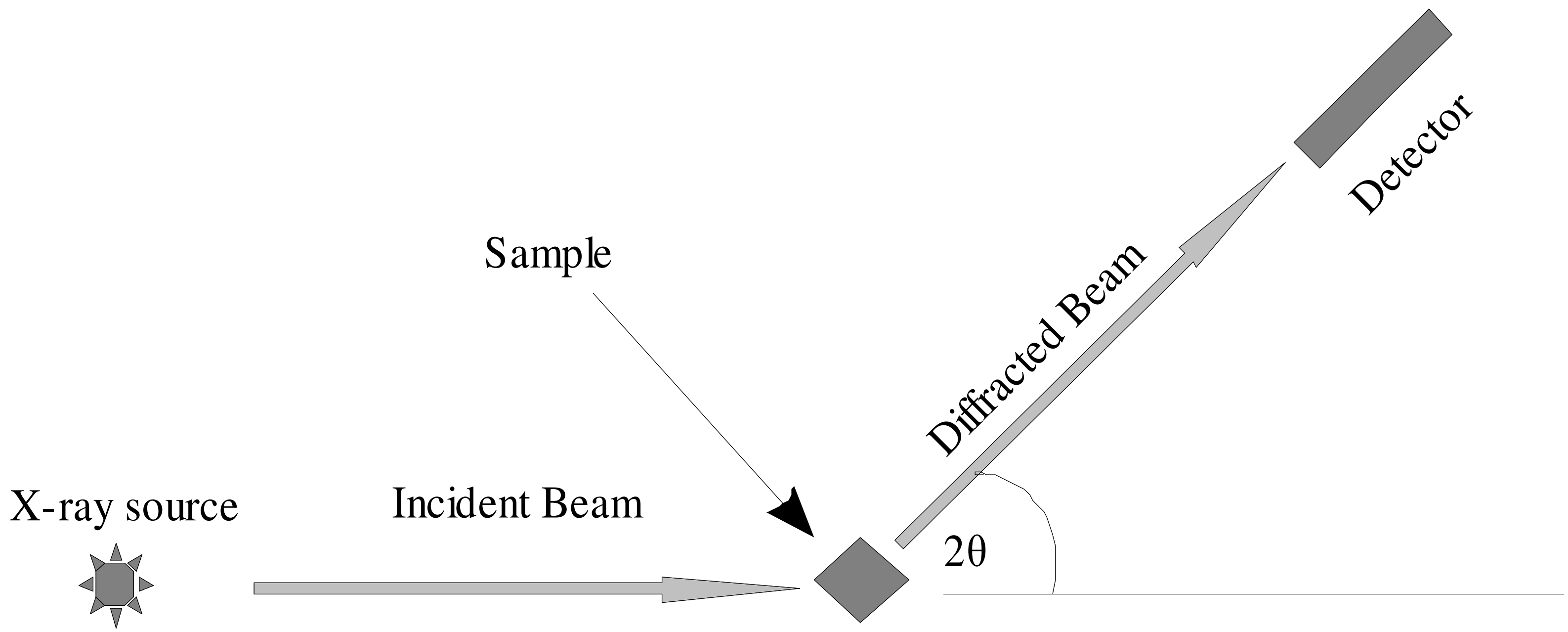
Abstract

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

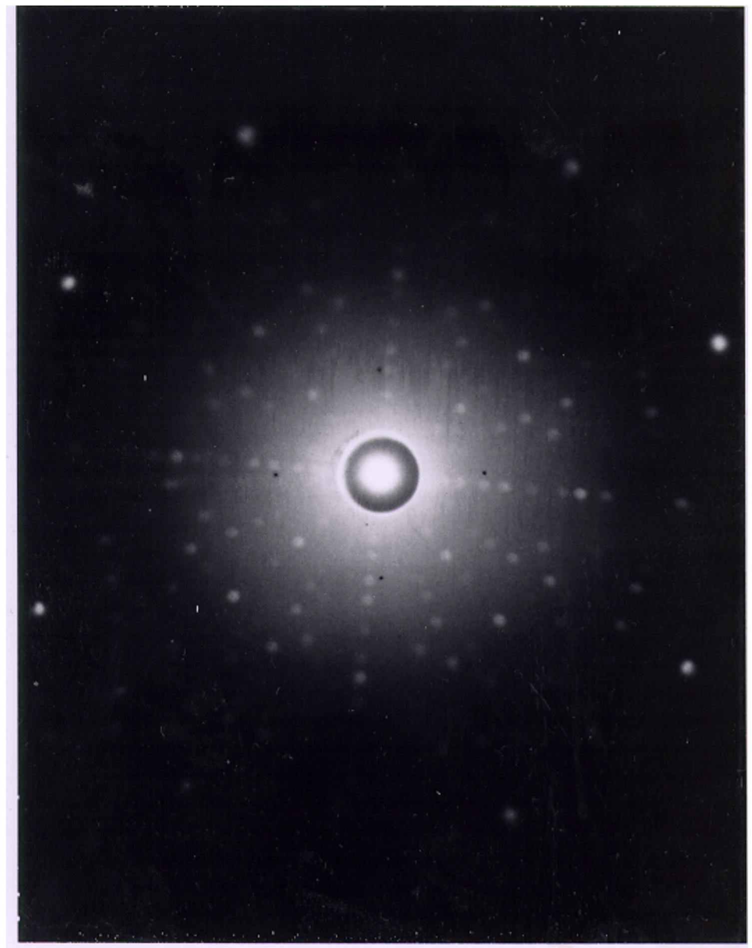
Outline

- Motivation and Introduction
- Verify Principles
  - Bragg’s Law
  - Scherrer Law
- Experimental Verification
- Switched beam design
- Conclusion and Further Work

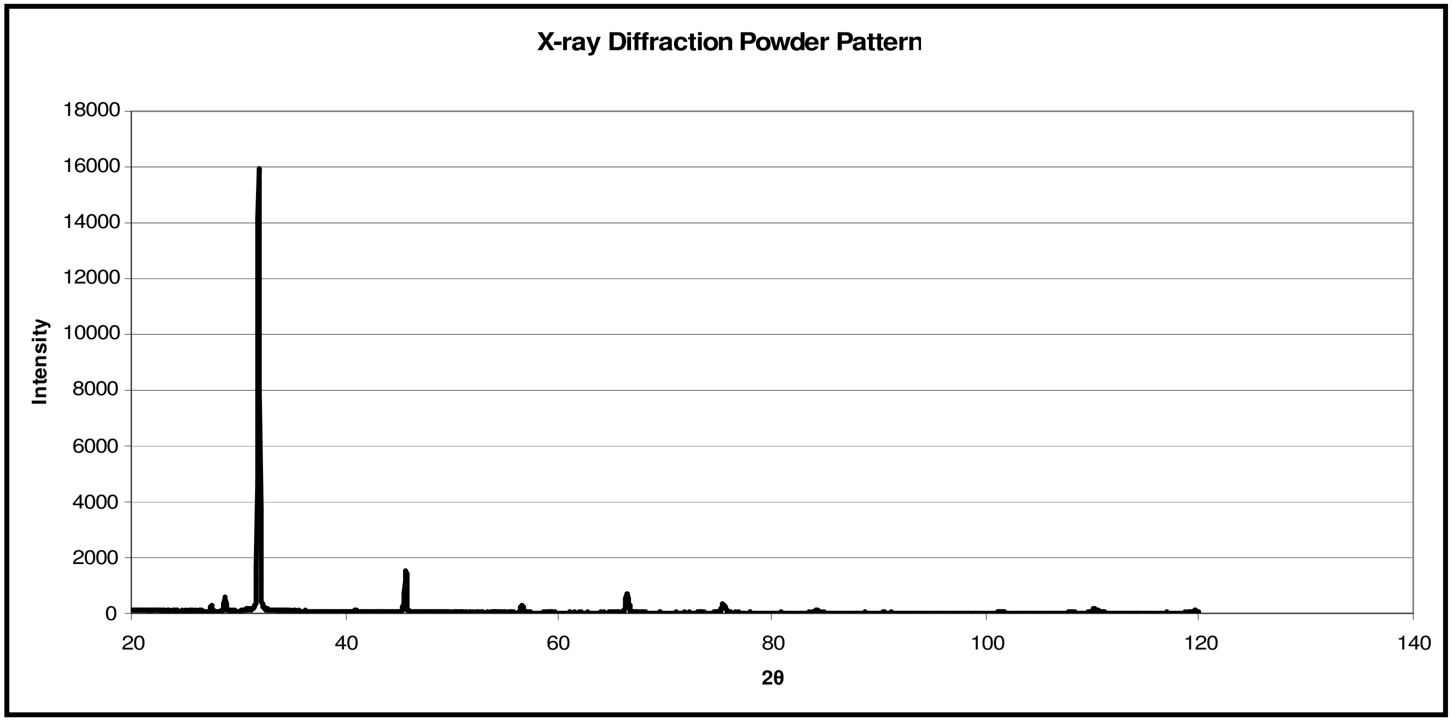
The Classic Experimental Setup



Some Typical Data…



Some Typical Data…

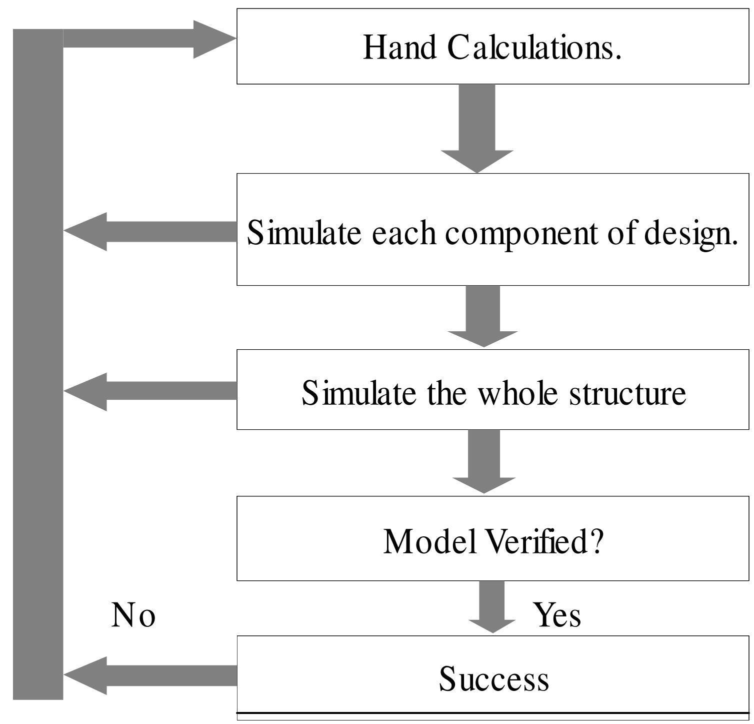


Principles of X-ray Diffraction

- Bragg's Law
- The Scherrer Equation
- The Reciprocal Lattice
- The Ewald Sphere
- The Scattering Factor

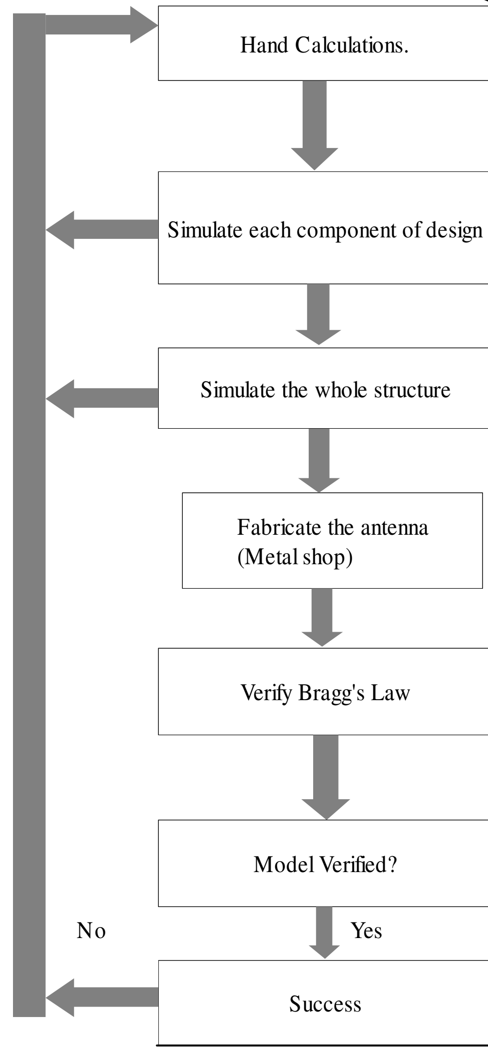
Motivation and Methodology

- 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

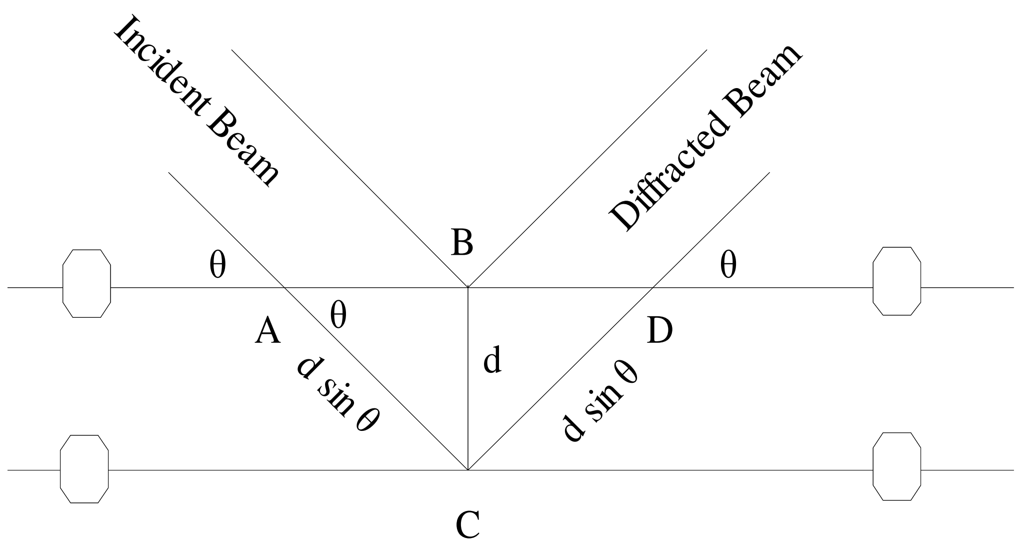
Antenna

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

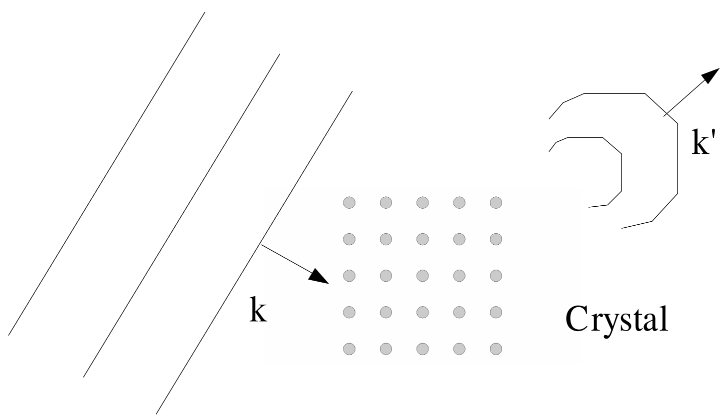
Direction of Main Lobe

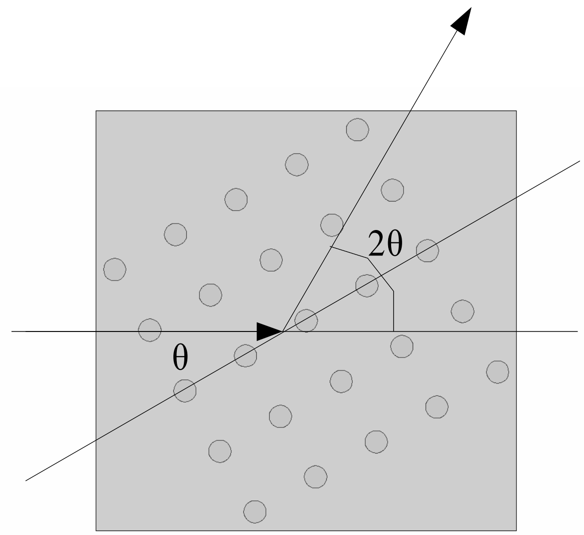
- The direction of the main lobe of the antenna is determined by Bragg's Law:

$$\lambda = 2d \sin \theta$$

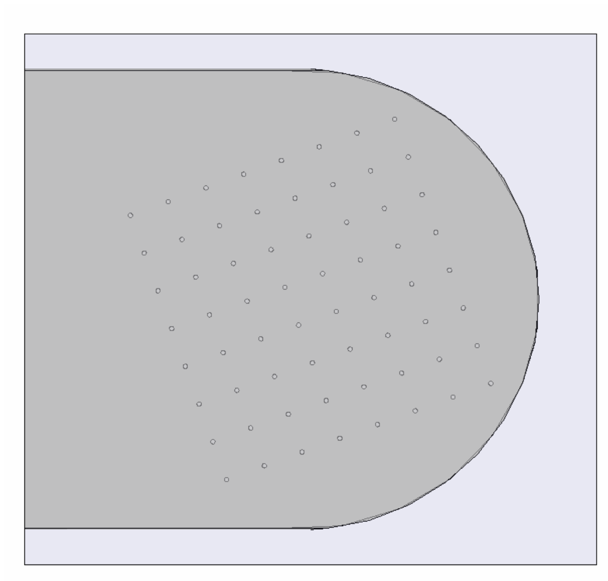


Sample Level View

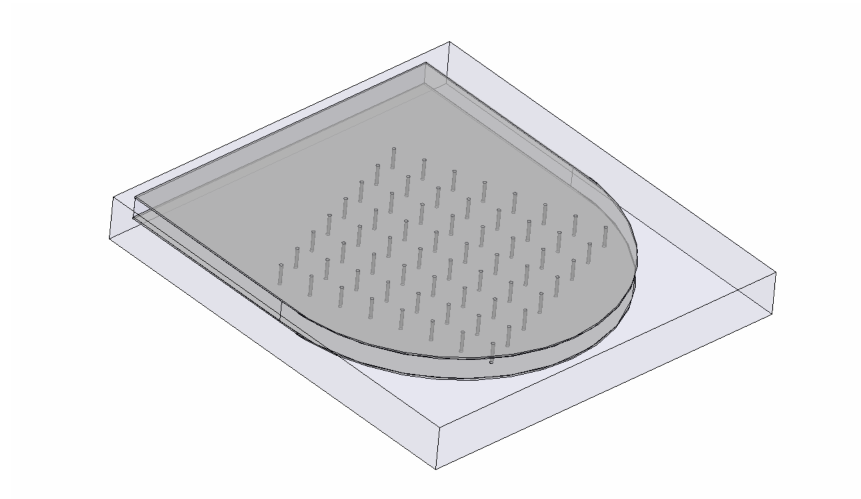




Bragg's Law Verified
Experimental Setup

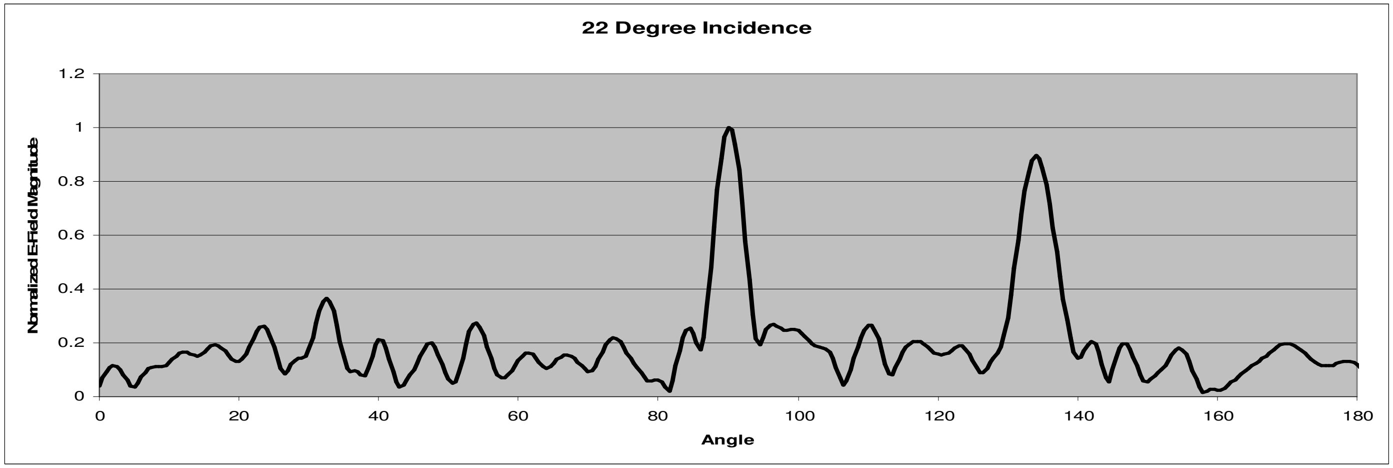


Top View

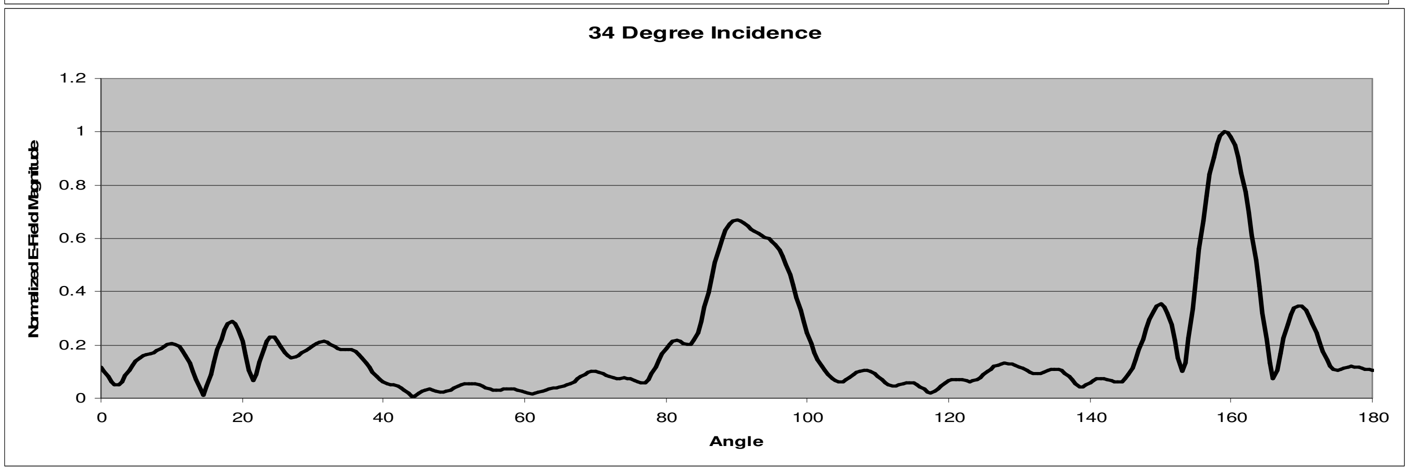


Skewed View

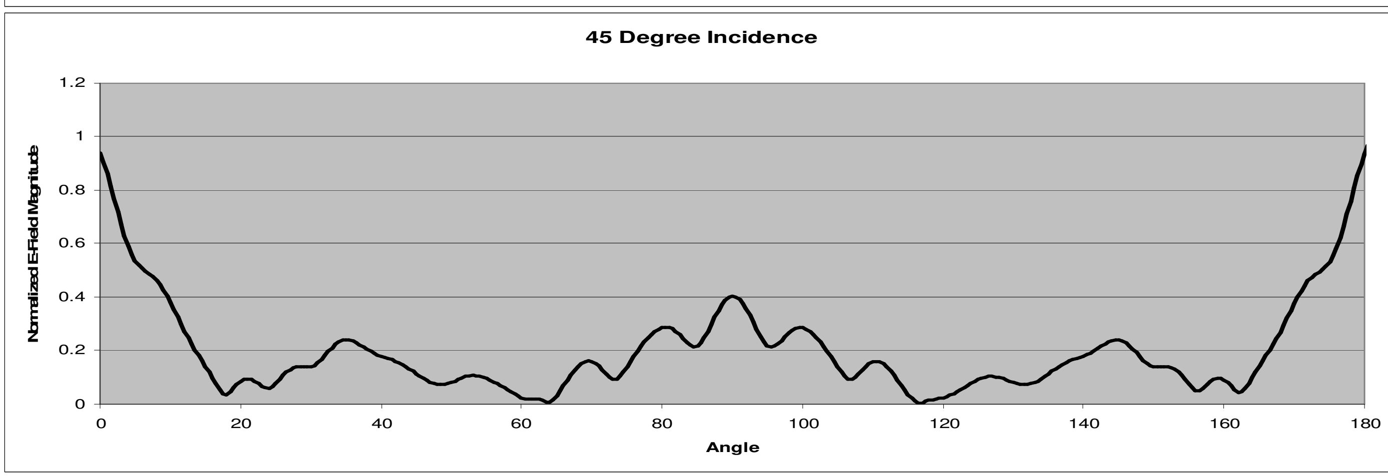
Results



22 Degree Incidence
Normalized E-Field Magnitude
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
120
140
160
180
Angle



34 Degree Incidence
Normalized E-Field Magnitude
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
120
140
160
180
Angle



45 Degree Incidence
Normalized E-Field Magnitude
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
120
140
160
180
Angle

Summary – Peak Locations

Predicted	Observed	
θ	(ϕ -90)/2	Δ
22	22	0.00%
24	24.25	0.40%
26	25.75	0.40%
28	27.75	0.30%
30	30	0.00%
32	32.25	0.30%
34	34.5	0.60%
36	37.25	1.50%
38	39	1.20%
40	41	1.20%
42	44.25	2.60%
44	44.5	0.60%
45	46	1.10%
46	46.75	0.80%
	Avg:	0.80%
	RSD	0.87

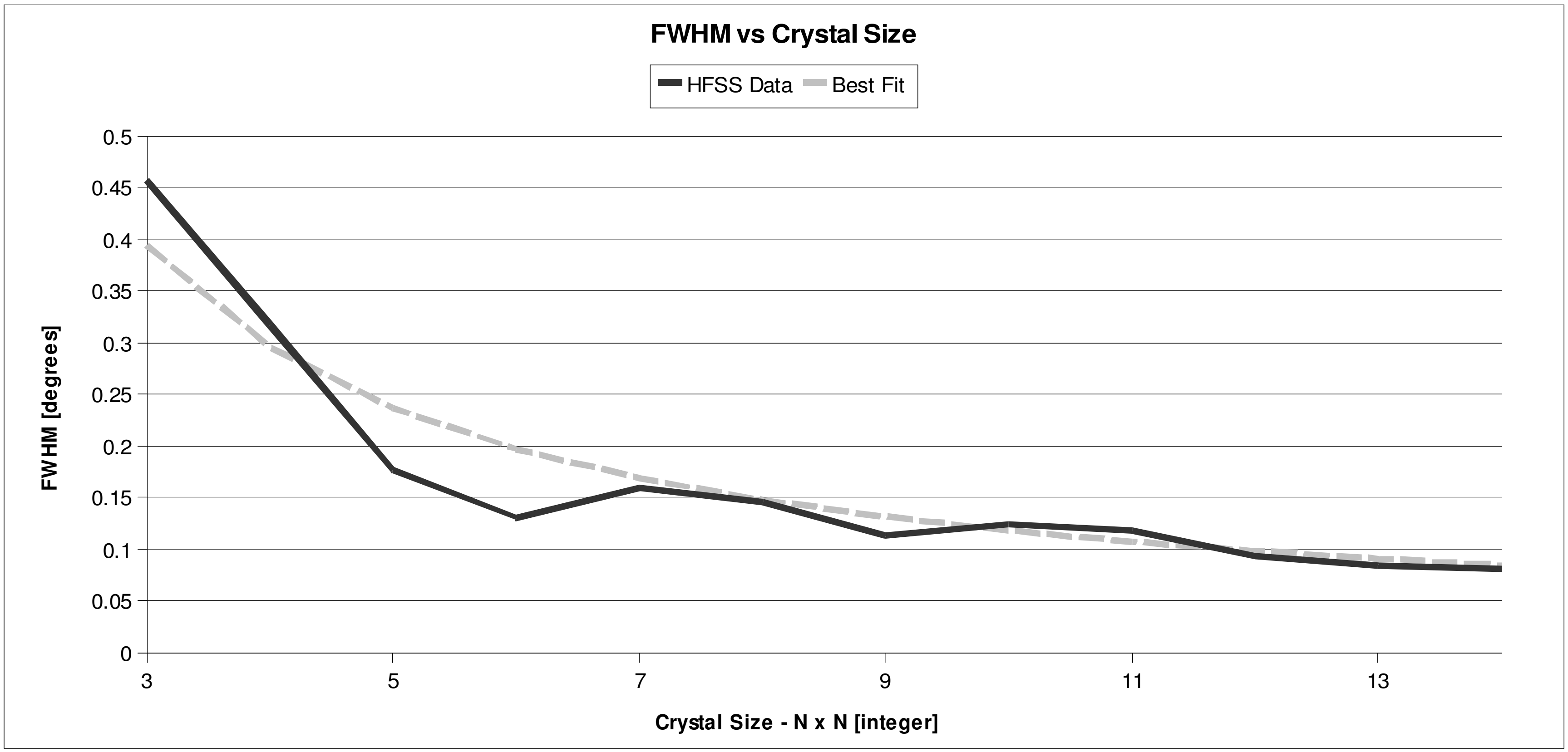
Beam Width

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

Verification

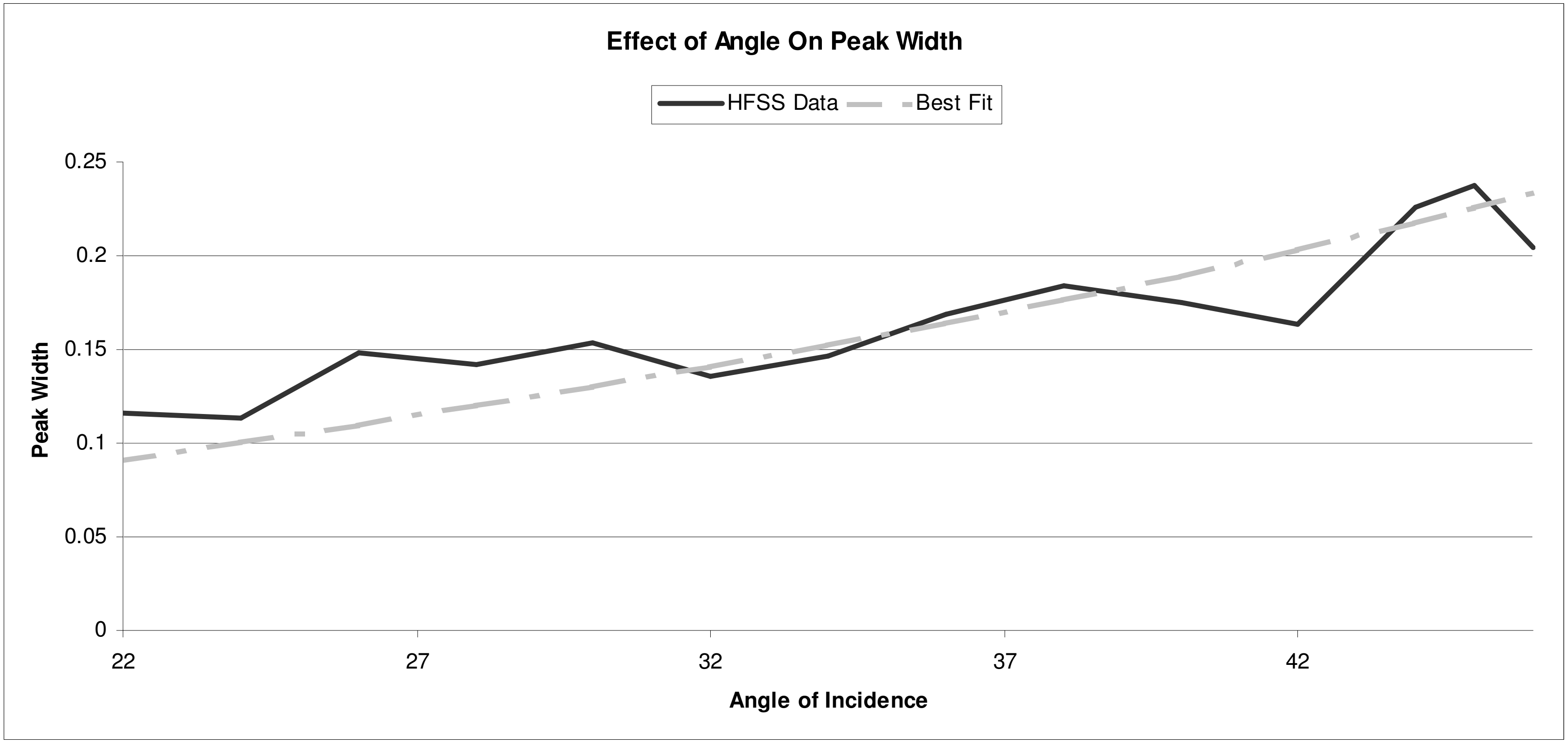
- The Scherrer law is verified in two ways
  - By varying N, holding all other quantities constant. Expect a 1/N dependence, and values of K on the order of unity.
  - Vary θ and a together; Use Bragg's Law to substitute for a in the Scherrer equation: $B(2\theta) = 2K \tan\theta / N$

Results



K = 1.02 Gave Best Fit

Results



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.

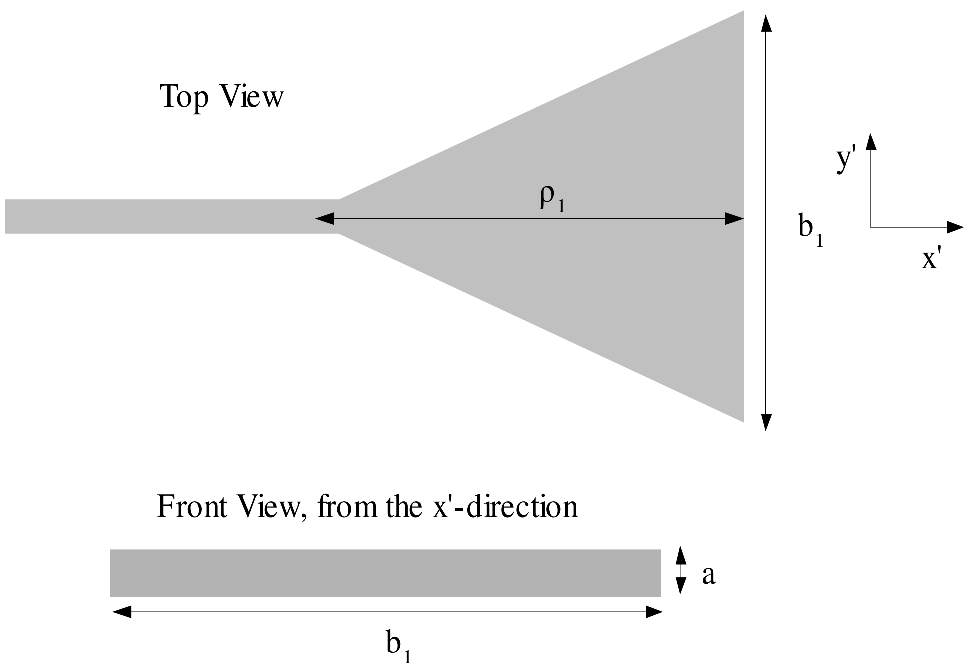
Experimental

- 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

Parameter	Value
OD	1.5" x 1.0"
ID	1.25" x 0.75"
f_{c10}	4.72 GHz
f_{c11}	9.17 GHz
Length	12"

Horn Section



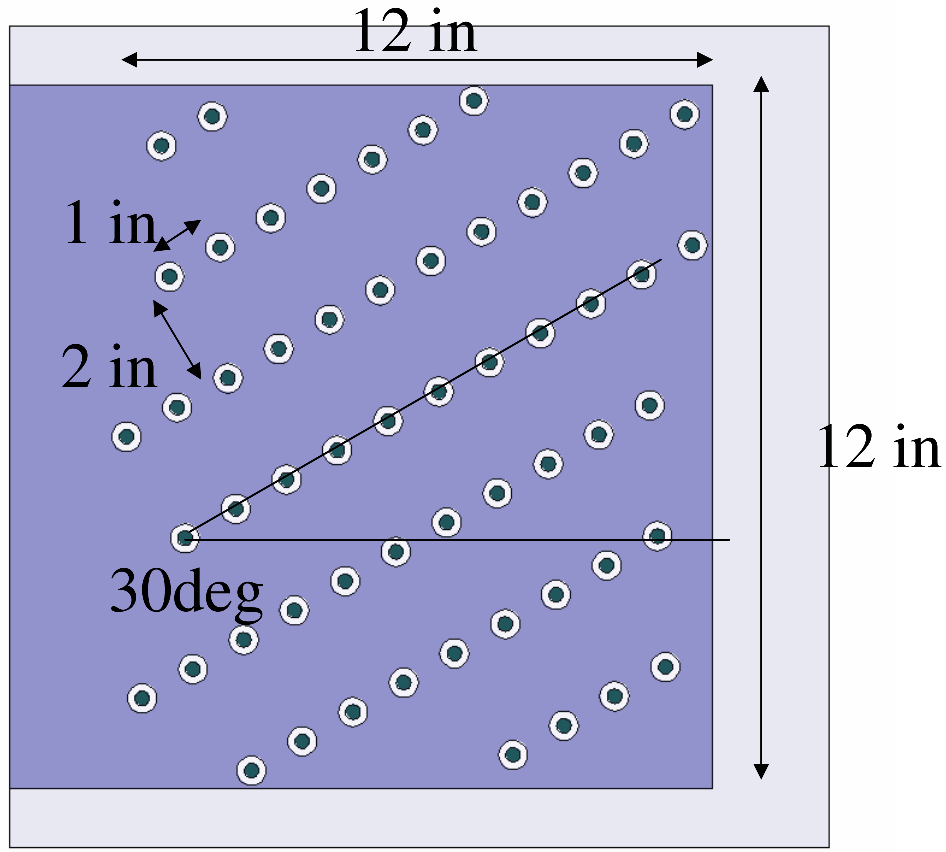
Parameter	Value
b_1	12"
a	1"
ρ_1	18"

Parallel Plate Section

d	1"
f_{c00}	0 GHz
f_{c10}	6 GHz

Crystal Section

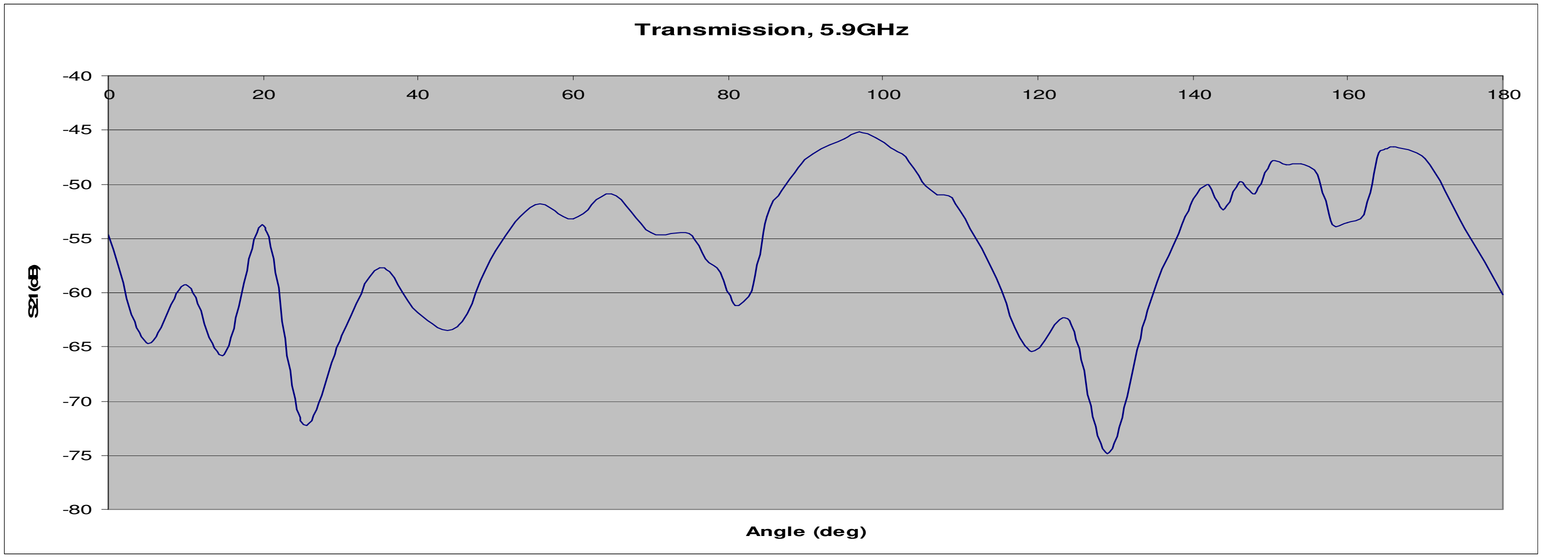
Post Diam	1/8"
θ	30^{o}
λ	2"

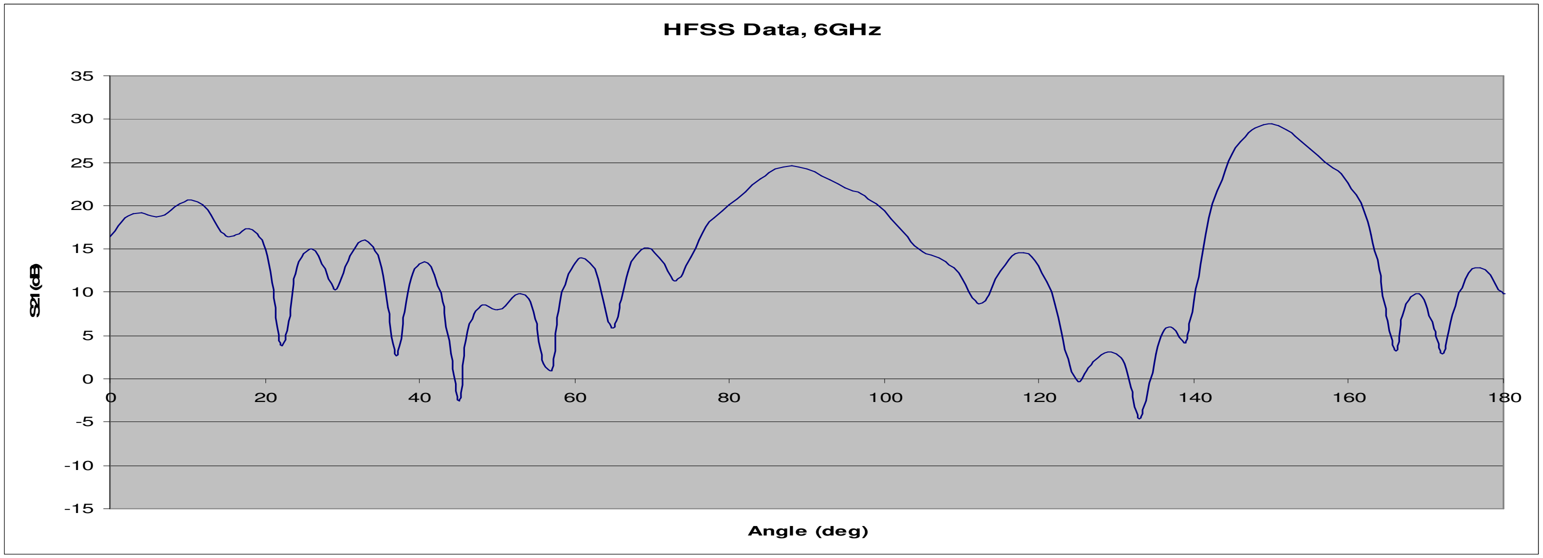


Results

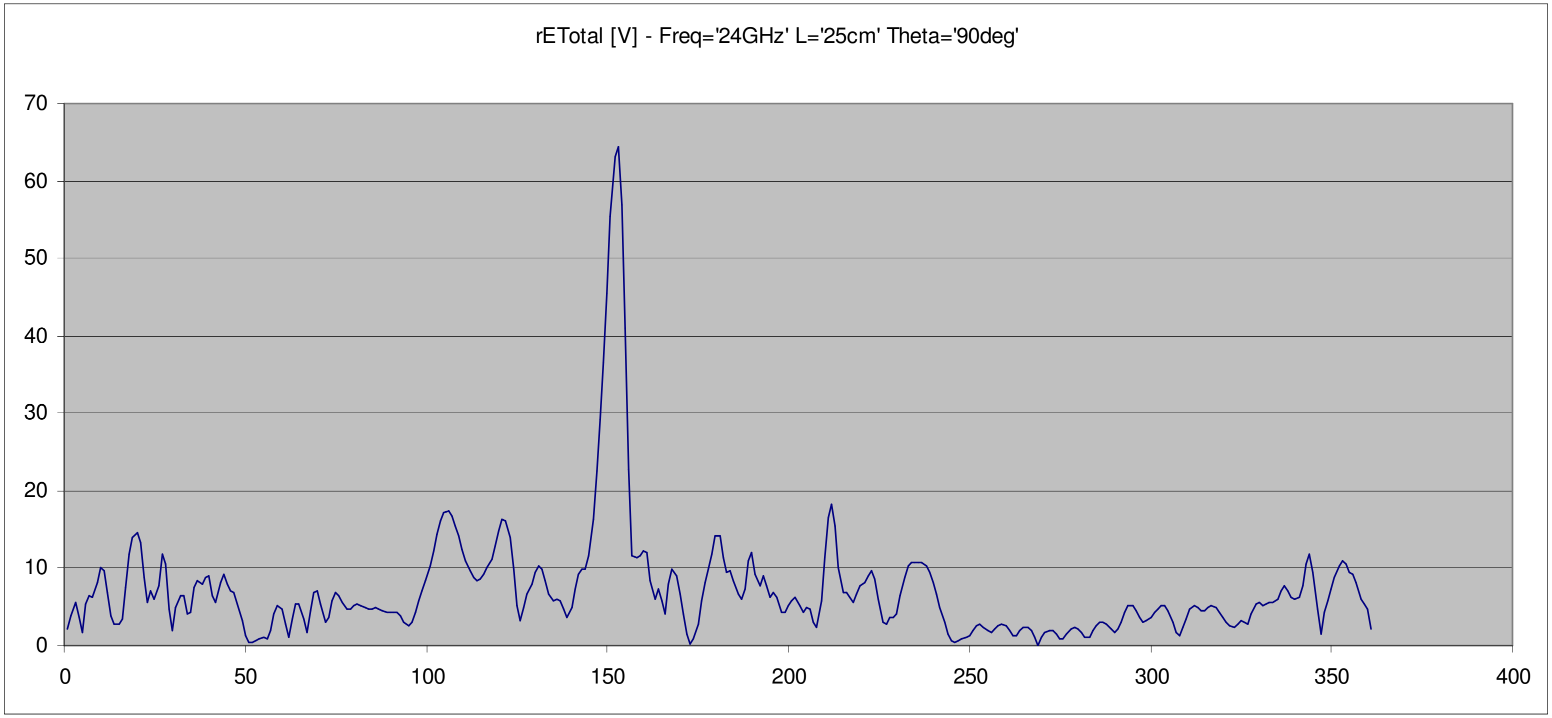
- Return Loss was better than –20dB at 5.9GHz, and was about –10dB at 6.223GHz
- 5.9GHz corresponds to a wavelength of 2in, but the best performance was obtained at 6.223GHz, with a gain over WR137 of 8dB

Results


Transmission, 5.9GHz
S21 (dB)
Angle (deg)
-40
-45
-50
-55
-60
-65
-70
-75
-80
0
20
40
60
80
100
120
140
160
180

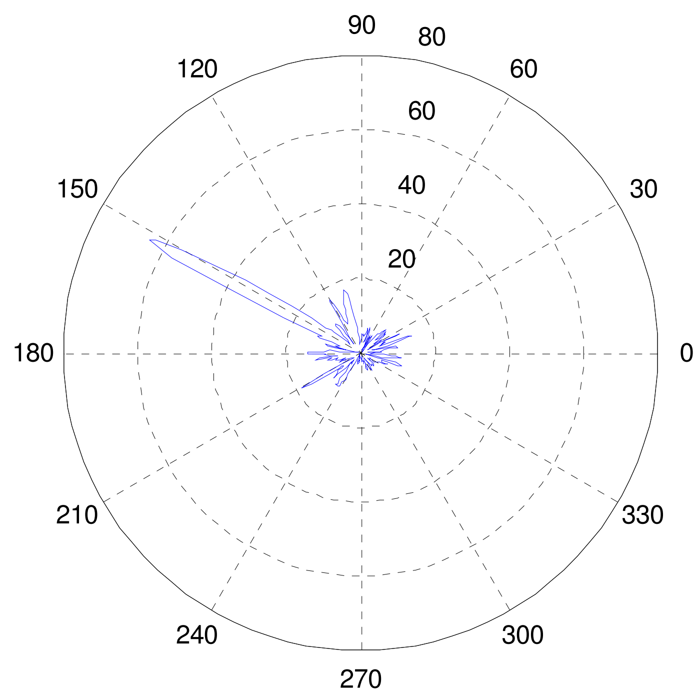

HFSS Data, 6GHz
S21 (dB)
Angle (deg)
35
30
25
20
15
10
5
0
-5
-10
-15
0
20
40
60
80
100
120
140
160
180

The best radiation pattern obtained

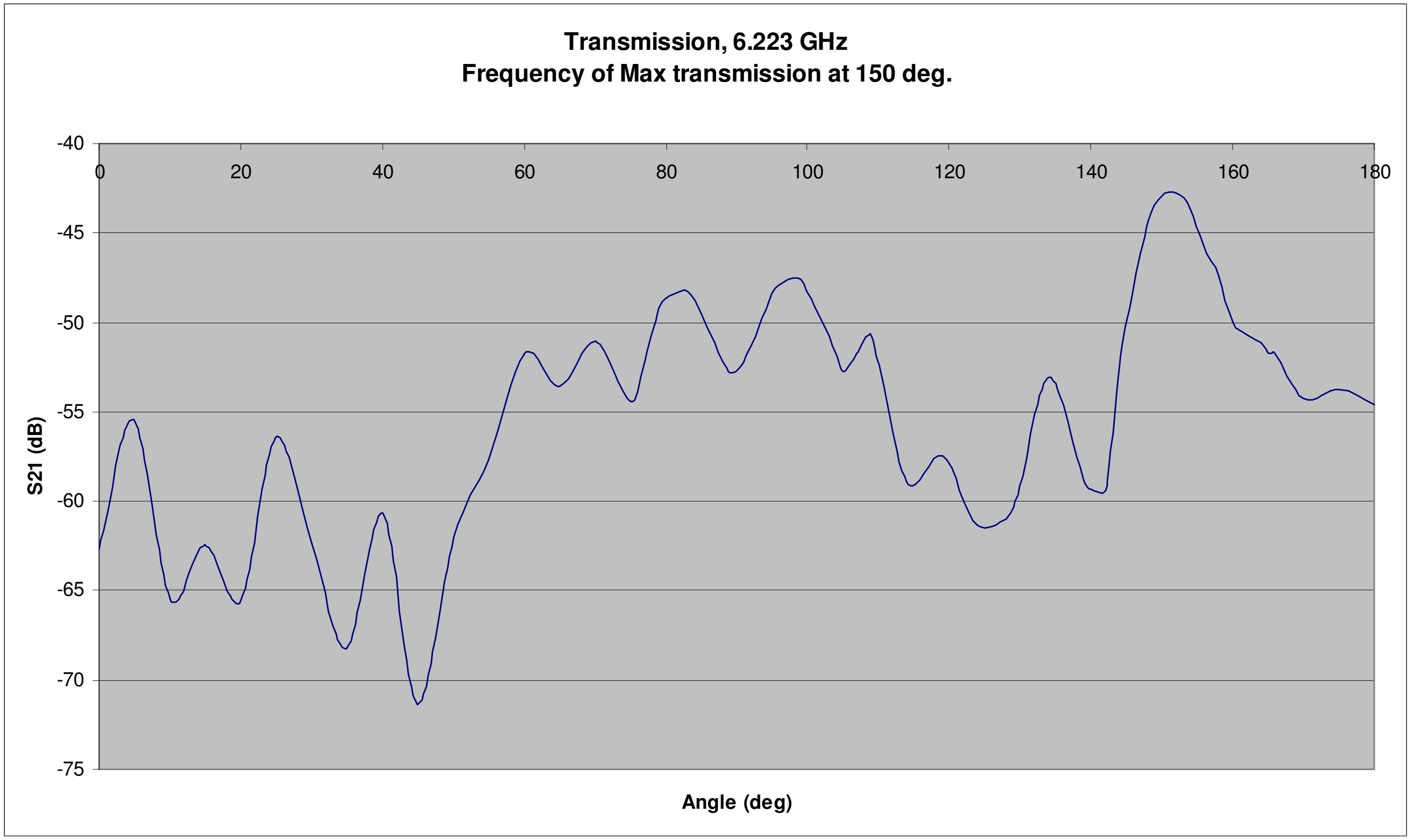


30 degree incidence

A polar plot



Results



Best Performance

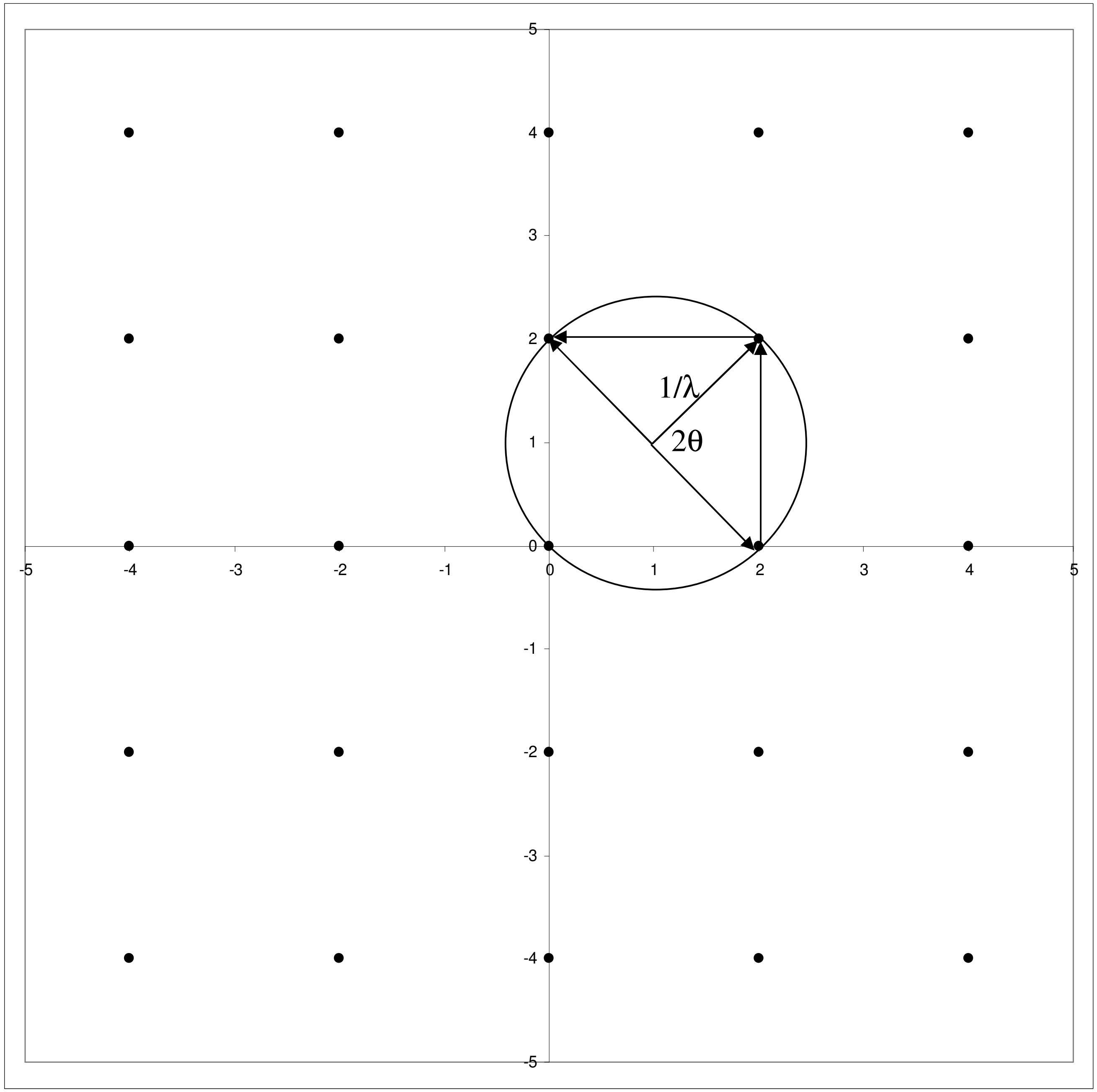
Conclusions and Observations

- Design could be improved with:
  - Better grounding
  - Higher quality plane wave.
  - Larger diameter posts
  - Longer interaction length

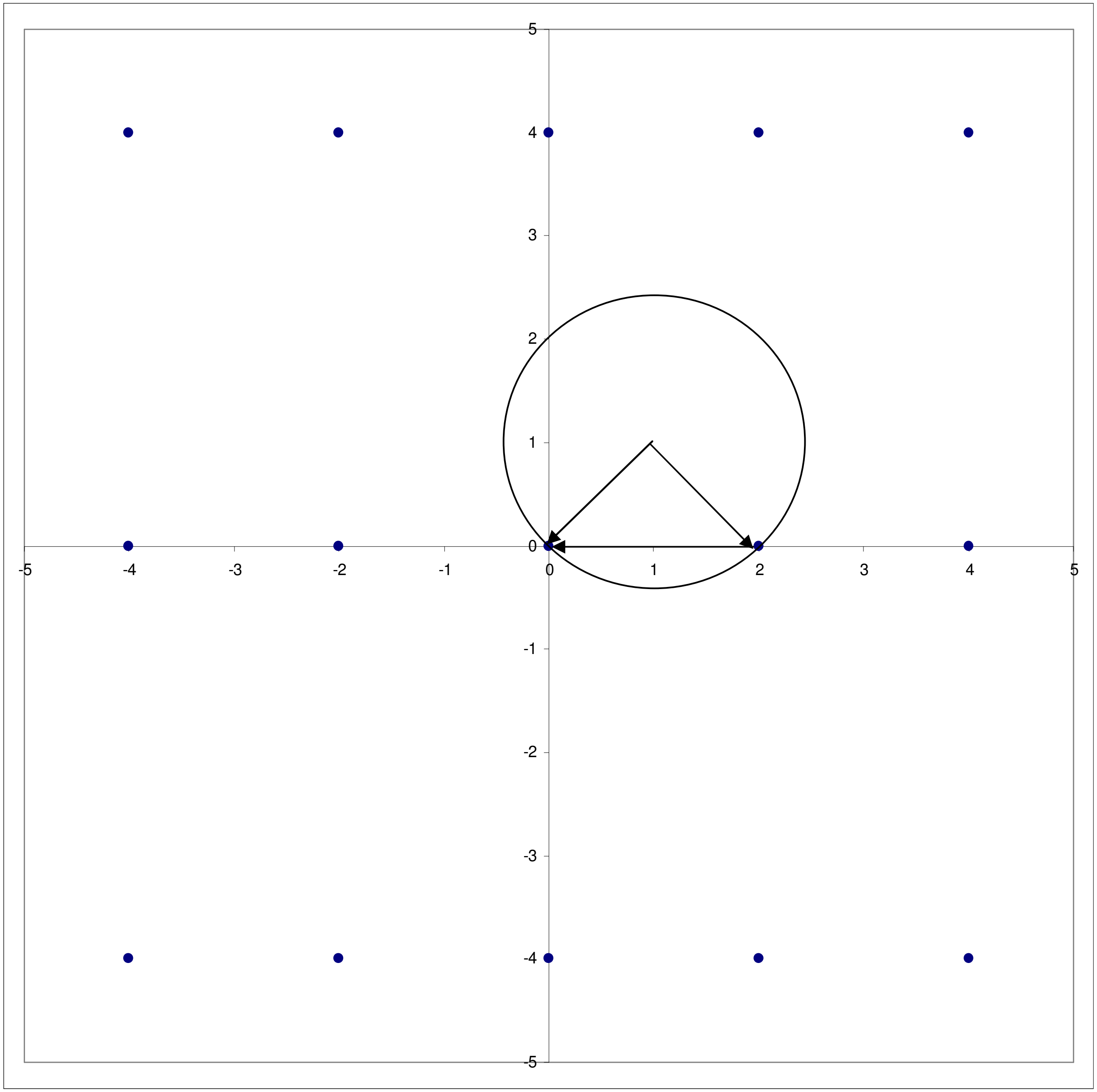
Switched Beam Antenna

- 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 1/a, 1/b.
- The “Ewald Circle” may be drawn in reciprocal space to describe an X-ray diffraction experiment, the circle having radius $1/\lambda$
- When the circle intersects two or more reciprocal lattice points, one or more reflections are created.

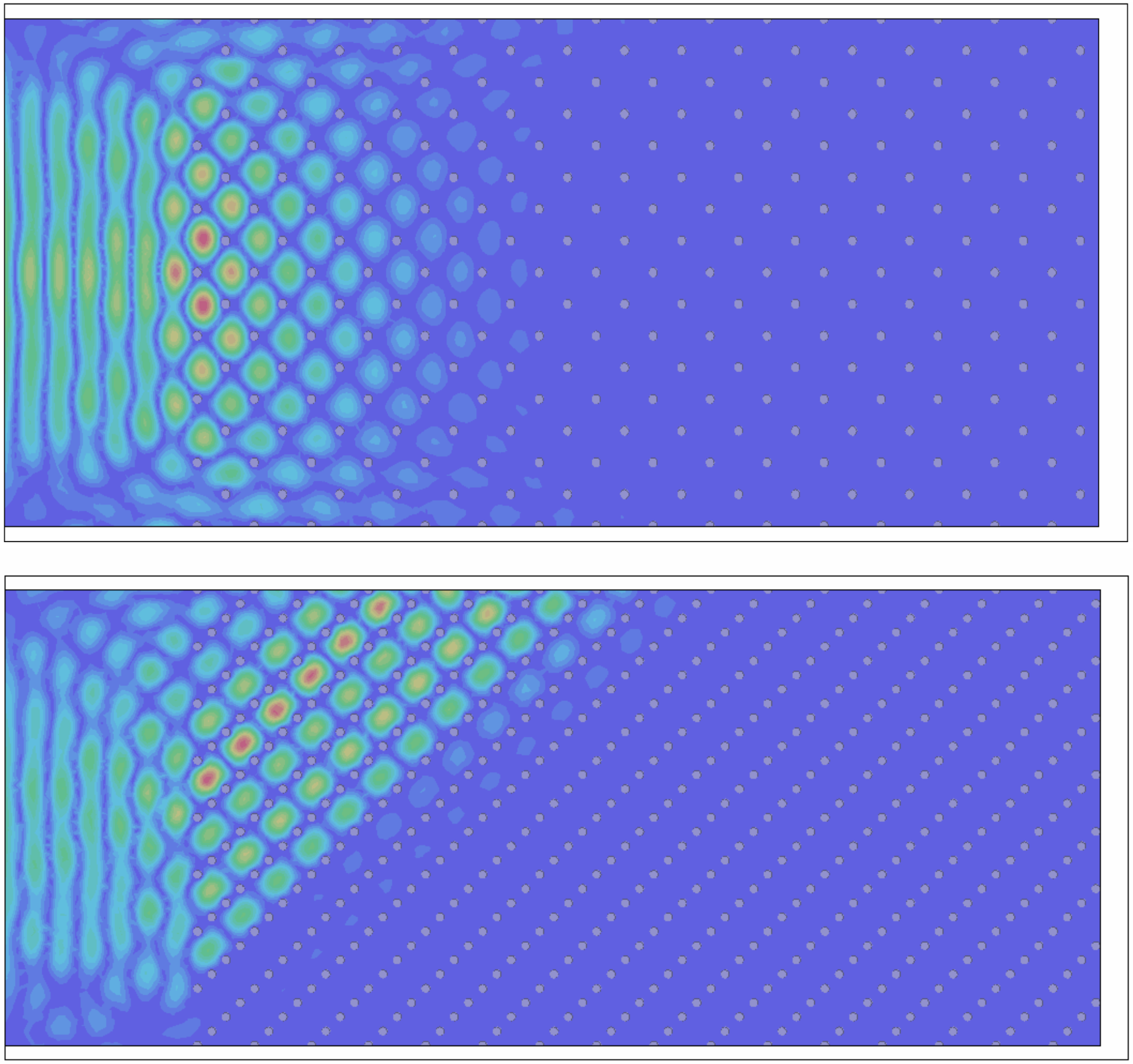
For the given diagram, there are two 45 degree reflections. If a = b = 0.5in, then λ = 0.707in



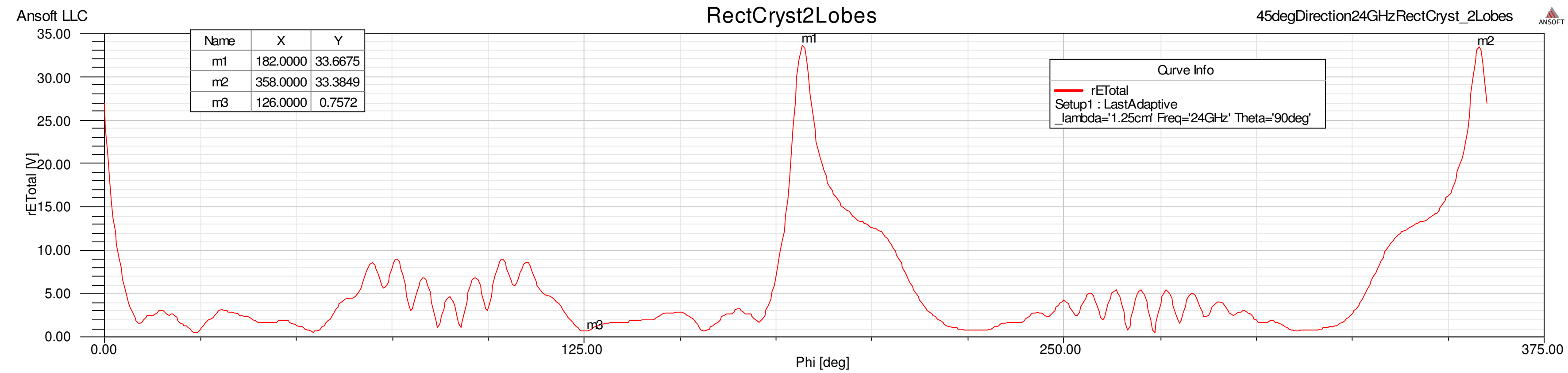
The reciprocal lattice has been altered by doubling the length of the basis vector in the vertical direction, corresponding to halving the direct-space lattice basis vector

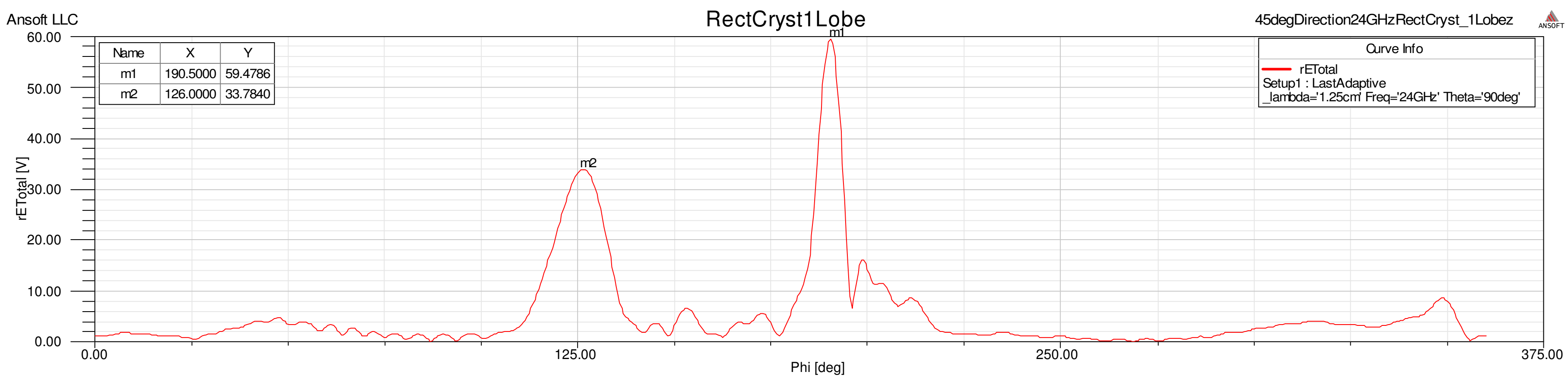


The two models



The two radiation patterns

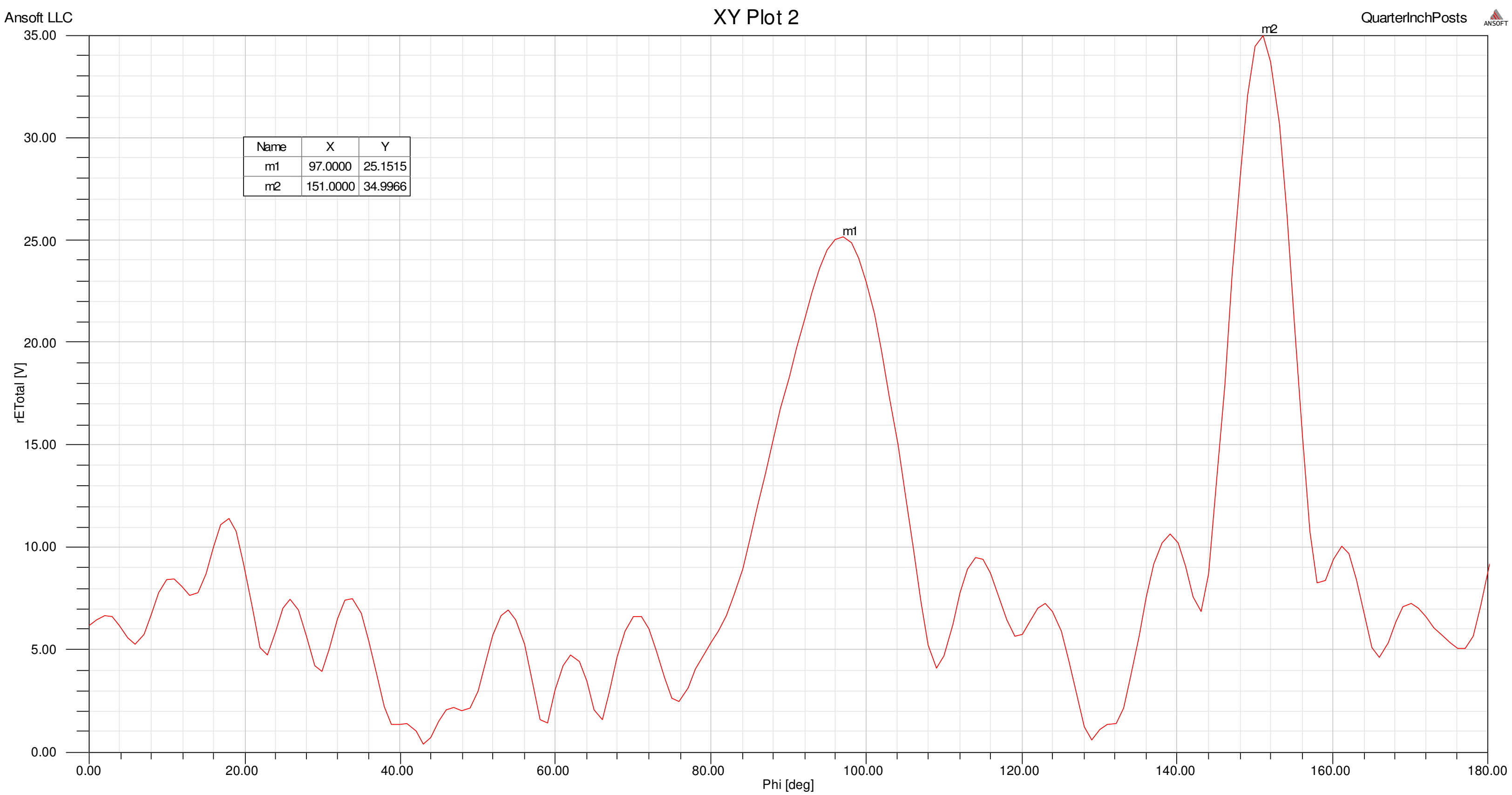




Conclusion

- 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



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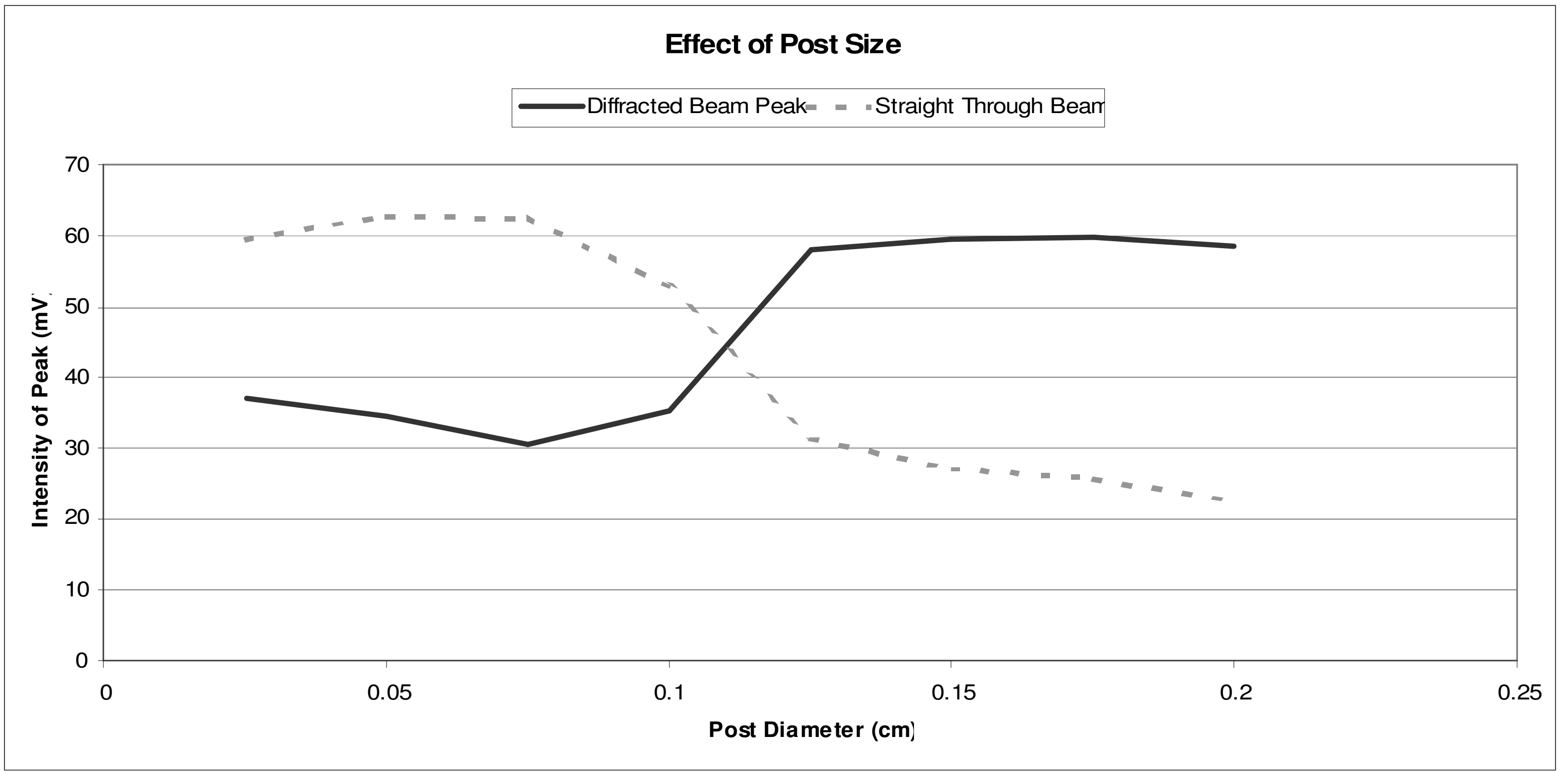
- Bill Shull of Zygo corporation, for helping with the construction of the antenna, and use of his Machine Shop,
- My Supervisor and co-workers at Space Systems Loral, for providing facilities and assistance to make the measurements.
- My Wife and family, for their patience with my seemingly endless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

Questions?

The effect of Post Diameter



Model Specifications

Parameter	Value
Plate Thickness - Top	0.1cm
Plate Thickness - Bottom	0.1cm
Plate Spacing	1.25cm
Crystal Size	8x8
Post Spacing	$\lambda/(2 \sin\theta)$
Post Radius	0.1cm
Angle of Incidence	22^o-46^o, 2^o steps; 45^o
Solution Frequency	24GHz
Max. ΔS	0.01