

# A Worked Example in 2-Dimensions

## Normal Lattice Space

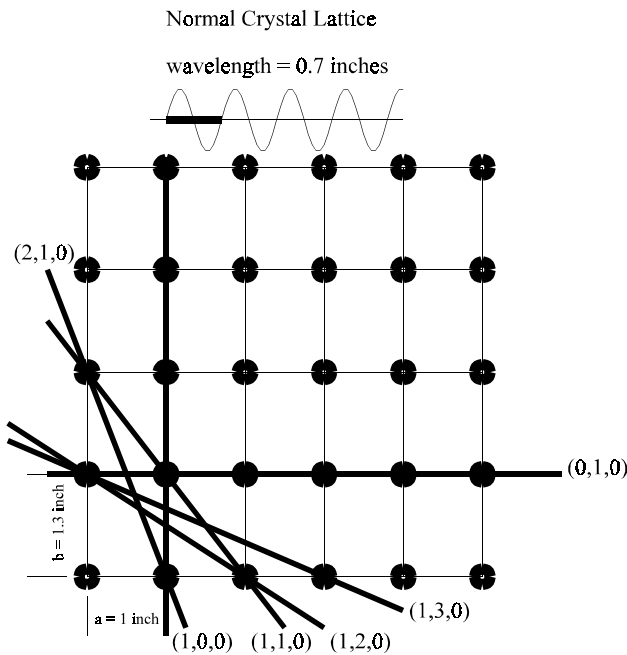
Starting information (ignoring the z-axis):

$$\begin{aligned} \lambda &= 0.7 \text{ inches,} \\ \vec{a} &= 1.0 \hat{i} \text{ inches,} \\ \vec{b} &= 1.3 \hat{j} \text{ inches,} \\ \vec{a} \perp \vec{b}, \quad \vec{a} \perp \vec{c}, \quad \vec{b} \perp \vec{c}. \end{aligned}$$

Miller's indices:

"Integer-ize"

Intercepts	Invert	to get index
$(1, \infty, \infty)$	$(1,0,0)$	$(1,0,0)$
$(\infty, 1, \infty)$	$(0,1,0)$	$(0,1,0)$
$(1, 1, \infty)$	$(1,1,0)$	$(1,1,0)$
$(1, 2, \infty)$	$(1, \frac{1}{2}, 0)$	$(2,1,0)$



## Reciprocal Lattice Space

Starting information:

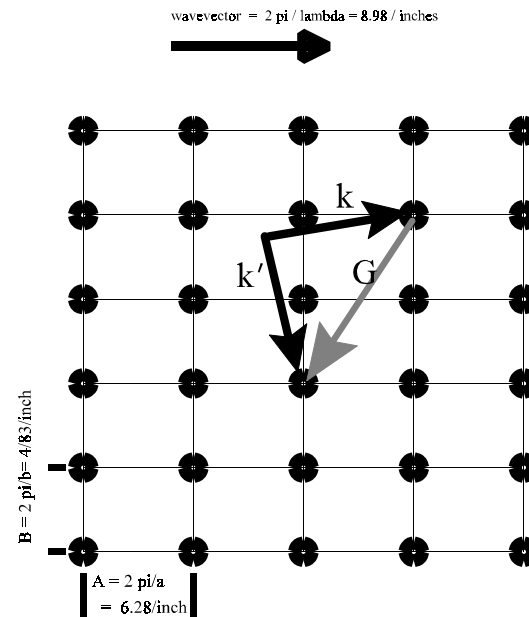
$$|\vec{k}| = \frac{2\pi}{\lambda} = 8.98 \text{ inch}^{-1},$$

$$\vec{A} = 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot \vec{b} \times \vec{c}} \quad \vec{B} = 2\pi \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot \vec{c} \times \vec{a}} \quad \vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot \vec{a} \times \vec{b}}$$

$$\vec{A} = \frac{2\pi}{a} \hat{i} = 6.28 \text{ inch}^{-1}, \quad \vec{B} = \frac{2\pi}{b} \hat{j} = 4.83 \text{ inch}^{-1}.$$

Also because it is an elastic scatter,  $|\vec{k}| = |\vec{k}'|$ , where  $\vec{k}$  is the incident wavevector and  $\vec{k}'$  is the diffracted wavevector.

### Reciprocal Crystal Lattice



## Normal

Condition for Bragg diffraction peak

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

OR

$$\theta = \arcsin \left( \frac{n \lambda}{2d} \right) .$$

Note: the range of  $n$  is limited to integers such that  $\theta$  is real.

**WHY??**

For diffraction from the (1,0,0) planes, the separation  $d = a = 1$  inch and one obtains:

n	$n\lambda / 2a$	$\theta$	$2\theta$
1	0.35	20.5	41
2	0.70	44.4	88.8
3	1.05		

Continue these calculations for the (0,1,0) series of planes.

For diffraction from the (1,1,0) planes, the separation

$d = ab / \sqrt{(a^2 + b^2)} = 0.79$  inch and one obtains:

n	$n\lambda / 2d$	$\theta$	$2\theta$
1	0.44	26.3	52.6
2	0.89	62.4	125
3	1.33		

Continue these calculations for the (2,1,0), (1,2,0), and (1,3,0) series of planes.

Do the planes with indices that have larger integers get closer or further apart?

Is there a maximum or a minimum distance,  $d$ , between reflecting plane beyond which interference will create "peaks?" If so what is it?

## Reciprocal

Condition for Bragg diffraction peak:

$$\begin{aligned} \Delta \vec{k} &= \vec{k}' - \vec{k} = \vec{G}, \\ \vec{G} &= m\vec{A} + n\vec{B}, \\ m, n &\text{ are integers.} \end{aligned}$$

One can find all of the scattering angles by construction (Called Ewald construction) First attach the head of  $\vec{k}$  to a lattice point, with its tail free to rotate, which is related to the crystal rotating in the incident beam. To the tail of  $\vec{k}$ , attach the tail of  $\vec{k}'$ . Place the head of  $\vec{k}'$  on a second lattice point and measure the angle between  $\vec{k}$  and  $\vec{k}'$ . This is the angle between the incident beam and the diffracted beam to a peak, and is equal to  $2\theta$ . Recall that  $\theta$  is the angle in the standard Bragg equation. The limiting condition on the integers  $m$  and  $n$  is that  $|\vec{G}| \leq 2|\vec{k}|$ . (Hint: When doing the Ewald's construction, one can work almost exclusively in the first quadrant.)

**WHY is the angle between  $\vec{k}$  and  $\vec{k}'$  equal to  $2\theta$ ?**

**WHY must  $|\vec{G}| \leq 2|\vec{k}|$ ?**

**Do the Ewald construction for this example crystal and verify the angles found on the left using  $2d \sin \theta = \lambda$ .**

So now to calculate the angle of diffraction peaks for a known crystal one can either use the Bragg equation directly or find the reciprocal lattice and do an Ewald construction. But that is not the problem at hand, which is the inverse problem. How does one start with the angles of the diffraction peaks and obtain the crystal's basis vectors? The basis vectors determine the spacing in the crystal and associated angles. This is often a dark art, but for simple 2D crystals it is not impossible.

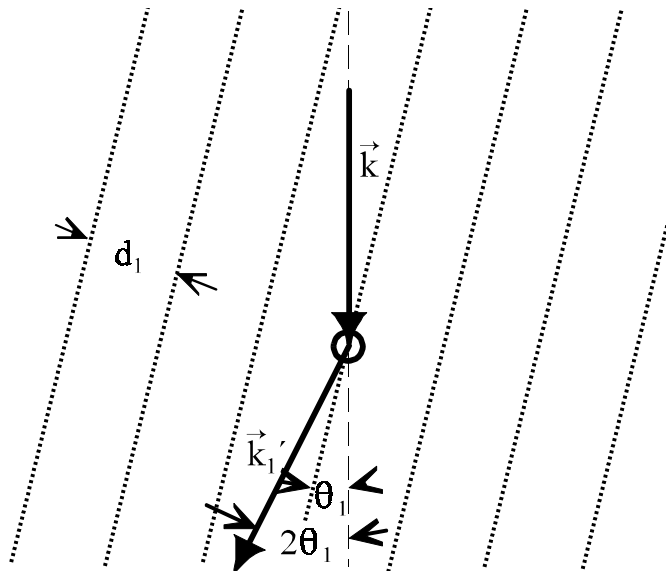
After making measurements, in a perfect world, one has a table of angles,  $2\theta$ , where a diffraction peak was observed. If we took measurements on our example crystal, we would have something like:

	<b>“Measured” Angles for Example Crystal Peaks and Analysis</b>									
Peak number	1	2	3	4	5	6	7	8	9	10
$2\theta^\circ$	31.2	41	52.6	65.2	81.1	88.8	97.2	108	123	125
$\theta^\circ$	15.6	20.5	26.3	32.6	40.5	44.4	48.6	53.9	61.7	62.4
$\sin(\theta) = n\lambda/2d$	0.27	0.35	0.44	0.54	0.65	0.70	0.75	0.81	0.88	0.89
<b>Analysis of Data for Crystal in Normal Space</b>										
$d/n = \lambda / (2 \sin\theta)$	1.3	1	0.80	$0.65 = 1.3 / 2$	0.54	$0.5 = 1 / 2$	0.47	$0.43 = 1.3 / 3$	$0.4 = 0.8 / 2$	$0.39 = 0.8 / 2$
Designation	S1	T1	U1	S2	V	T2	W	S3	U2'	U2''
Miller( not known before completing analysis)	010	100	110	010	120	100	210	010	130	110
<b>Analysis of Data for Crystal in Reciprocal Lattice Space</b>										
Reciprocal lattice separation $\equiv G$	4.85	6.29	7.90	9.70	11.67	12.57	13.47	14.55	15.80	15.98
Designation	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$	$G_6$	$G_7$	$G_8$	$G_9$	$G_{10}$

## Normal

In normal space, one can determine the direction normal to the reflecting planes, because the normal bisects the angle between the incident beam and the diffracted beam. The angular data along with the known wavelength of the microwave, allows one to calculate  $d/n$ . In this data, look for multiples, to help determine  $n$  and thus  $d$ . It may take several, iterations of guessing and testing. It is possible the  $n = 1$  peak is blended with other peaks and not resolved for small diffraction angles.

For each diffraction peak one plane separation,  $d$ , and an angle,  $\theta$ . One can draw a series of parallel lines, each a distance  $d$  from the next. The angles at which these lines are drawn take a bit more thought. If done correctly, the intersection of the various lines one series with the other, should indicate the location of the scattering centers. Start by picking the angle of the incident microwaves, say vertically down, and an origin where one scatterer is located. Starting with the peak associated with the largest plane separation ( that is peak # 1, in this example) draw the first line through the origin and an angle  $\theta$  relative to the incident microwaves.



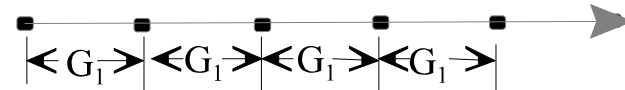
## Reciprocal

In reciprocal lattice space, the trick for converting scattering angles to lattice structure goes like this. First find the separations, denoted  $G$ , between individual lattice points in the reciprocal lattice. In the Ewald construction one has an isosceles with 2 sides of length  $|\vec{k}|$  with a common angle,  $\theta$ . The unequal side has a length,  $G = |\vec{G}|$  and it is straightforward to show that:

$$2|\vec{k}| \sin \theta = G .$$

First choose a one point or origin, and a direction. (These may be chosen randomly, but wisdom suggest starting near the lower left and choosing either a vertical or horizontal direction. ) Your chosen point is one lattice point. A second lattice point is a distance  $G_1$  from the origin in your chosen direction. In this same direction one can repeat this process to construct a series of lattice points along a line a distance  $G_1$  apart

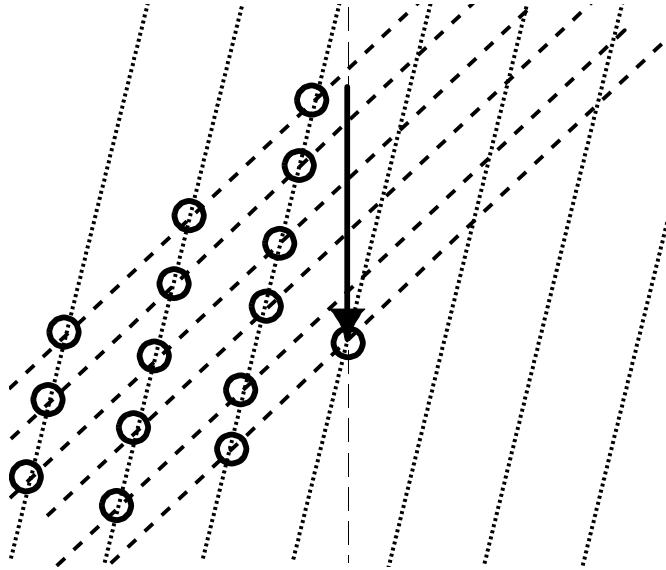
The first step in recreating the reciprocal lattice.



From each of these points scribe arcs with radii equal to the other known  $G$ 's. The intersections of the arcs MAY indicate a new lattice point. Note intersections less than  $G_1$  away from the first set of points probably are not lattice points because they would result in an even shorter  $G$ , unless somehow a peak was missed. With luck, a missed diffraction peak will be apparent. For example if you you have  $G$ 's of length 2 and 3 you might want to check to see if a  $G$  of length 1 was missed. A bit of trial and error and a few iterations and one can get a fair match to the reciprocal lattice.

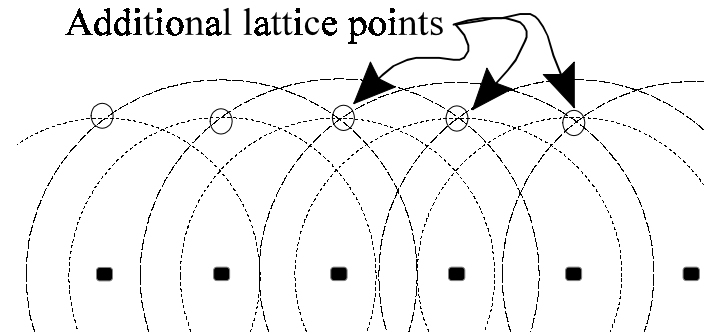
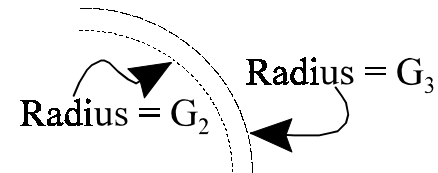
## Normal

So the first set of parallel lines is easy. A problem arises when one naively repeats the process for peak # 2 on the same figure. The problem is that the scattering planes are about  $90^\circ$  from where they belong relative to the first set of lines. But things work better working with information from peak # 3.



Basically this is mostly guess work, trying some combination and then testing to see if everything works. Using overlays like overhead transparencies may help. If the crystal is square (or equal length sided parallelogram), then two different sets of planes produce peaks at the same angle. Dealing with this degeneracy may be tricky.

## Reciprocal



With a second row of lattice points for the reciprocal lattice, one has the basis vectors,  $\vec{A}$  and  $\vec{B}$ . From these the entire reciprocal lattice can easily be generated. The trick is to get back to the real lattice.

$$\vec{a} = 2\pi \frac{\vec{B} \times \vec{C}}{\vec{A} \cdot (\vec{B} \times \vec{C})}$$

$$\vec{b} = 2\pi \frac{\vec{C} \times \vec{A}}{\vec{B} \cdot (\vec{C} \times \vec{A})}$$

$$\vec{c} = 2\pi \frac{\vec{A} \times \vec{B}}{\vec{C} \cdot (\vec{A} \times \vec{B})}$$

Note by definition  $\vec{a} \perp \vec{B}$  and  $\vec{b} \perp \vec{A}$ , so the angles are easy.