Today's Outline - October 19, 2016

Today's Outline - October 19, 2016

- Final presentation

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- Ewald sphere (continued)

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- Modulated Structures

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Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Monday, October 24, 2016

Today's Outline - October 19, 2016

- Final presentation
- Ewald sphere (continued)
- Modulated Structures
- Crystal Truncation Rods
- Diffuse Scattering
- Debye-Waller factor

Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Monday, October 24, 2016

Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Wednesday, November 2, 2016

No class on Wednesday, November 9, 2016

Final presentation

1. Choose paper for presentation

Final presentation

1. Choose paper for presentation
2. Clear it with me!

Final presentation

1. Choose paper for presentation
2. Clear it with me!
3. Do some background research on the technique

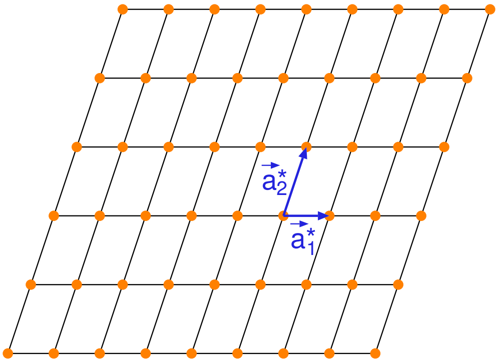
Final presentation

1. Choose paper for presentation
2. Clear it with me!
3. Do some background research on the technique
4. Prepare a 15 minute presentation

Final presentation

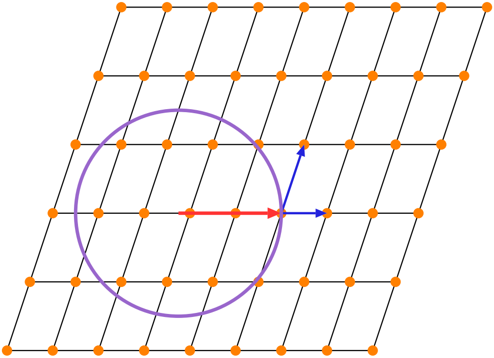
1. Choose paper for presentation
2. Clear it with me!
3. Do some background research on the technique
4. Prepare a 15 minute presentation
5. Be ready for questions!

Ewald sphere & the reciprocal lattice



The reciprocal lattice is defined by the unit vectors $\vec{a}_1^*$ and $\vec{a}_2^*$.

Ewald sphere & the reciprocal lattice



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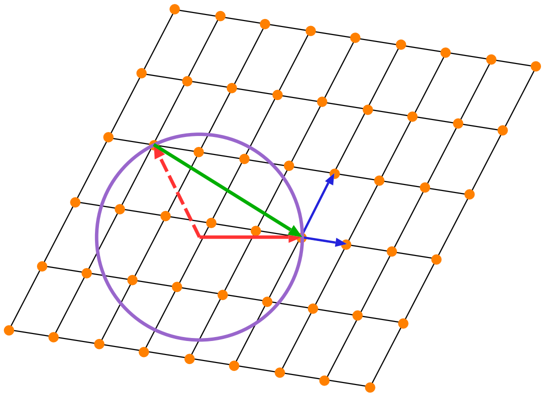
The key parameter is the relative orientation of the incident wave vector $\vec{k}$

Ewald sphere & the reciprocal lattice



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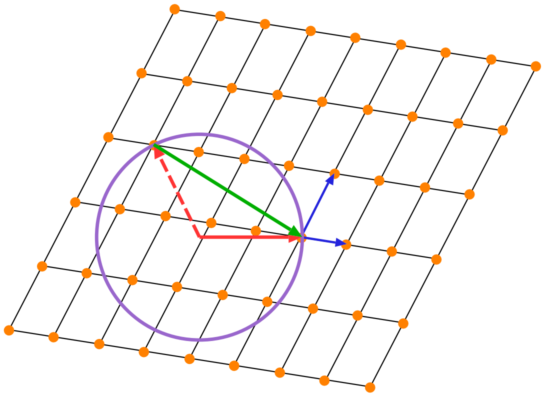
As the crystal is rotated with respect to the incident beam, the reciprocal lattice also rotates

Ewald sphere & the reciprocal lattice



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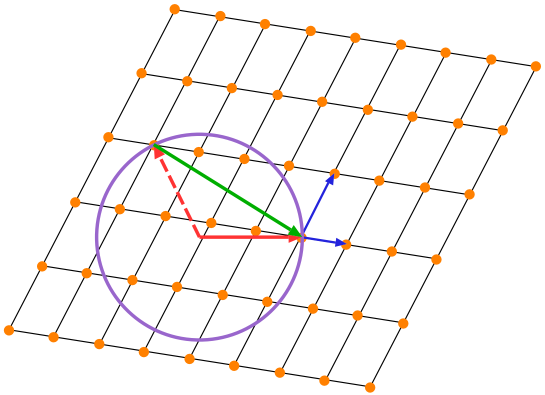
When the Ewald sphere intersects a reciprocal lattice point there will be a diffraction peak in the direction of the scattered x-rays.

Ewald sphere & the reciprocal lattice



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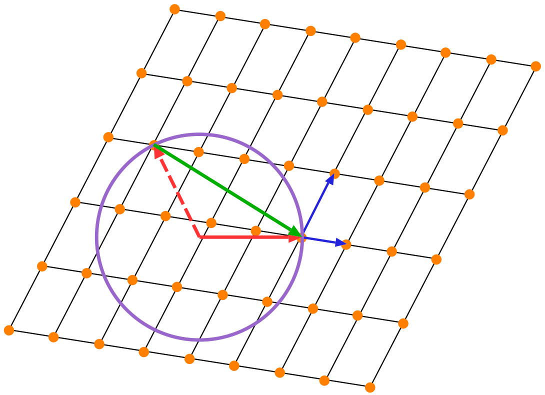
Ewald sphere & the reciprocal lattice



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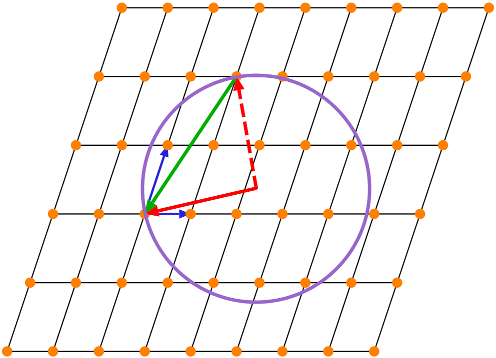
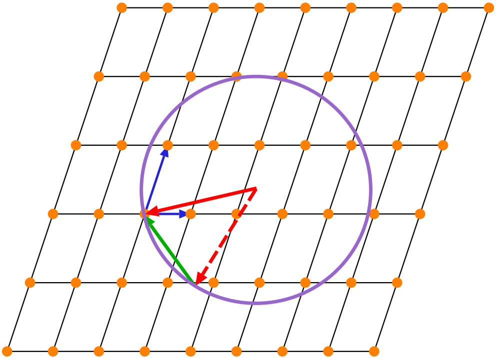
$$\vec{G}_{hlk} = h\vec{a}_1^* + k\vec{a}_2^*$$

Ewald construction



It is often more convenient to visualize the Ewald sphere by keeping the reciprocal lattice fixed and “rotating” the incident beam to visualize the scattering geometry.

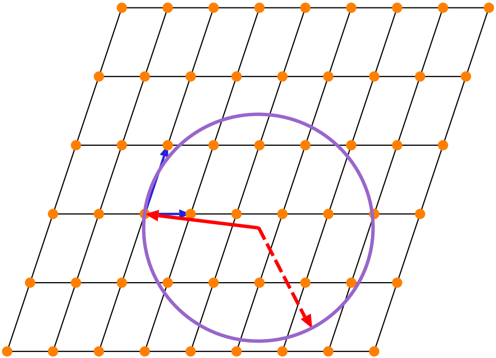
Ewald construction



It is often more convenient to visualize the Ewald sphere by keeping the reciprocal lattice fixed and "rotating" the incident beam to visualize the scattering geometry.

In directions of $\vec{k}'$ (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.

Ewald construction

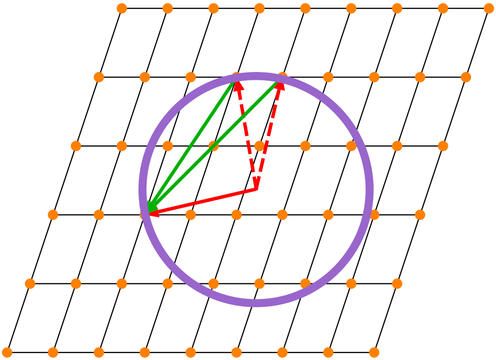


It is often more convenient to visualize the Ewald sphere by keeping the reciprocal lattice fixed and "rotating" the incident beam to visualize the scattering geometry.

In directions of $\vec{k}'$ (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.

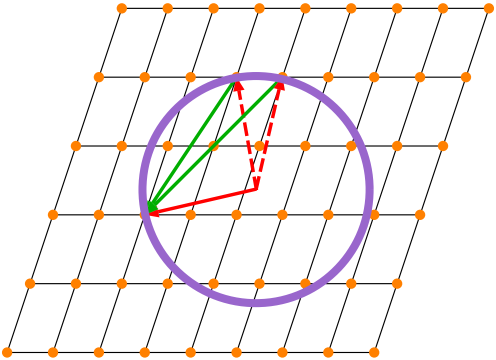
If the crystal is rotated slightly with respect to the incident beam, $\vec{k}$, there may be no Bragg reflections possible at all.

Polychromatic radiation



If $\Delta\vec{k}$ is large enough, there may be more than one reflection lying on the Ewald sphere.

Polychromatic radiation



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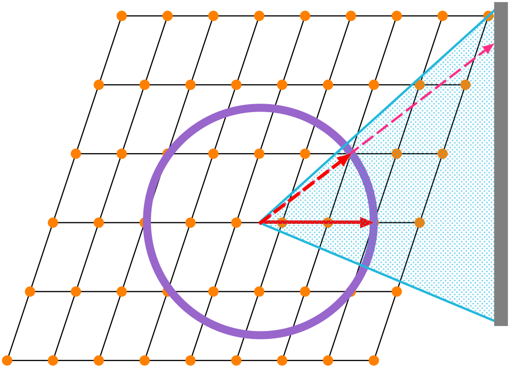
With an area detector, there may then be multiple reflections appearing for a particular orientation (very common with protein crystals where the unit cell is very large).

Polychromatic radiation



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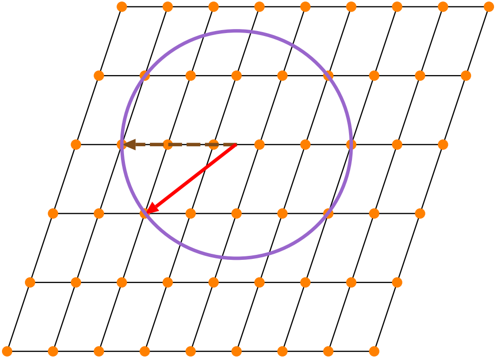
With an area detector, there may then be multiple reflections appearing for a particular orientation (very common with protein crystals where the unit cell is very large).

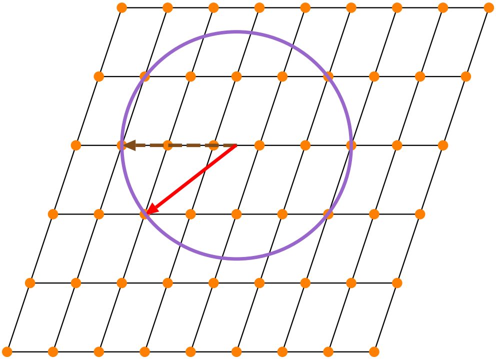
In protein crystallography, the area detector is in a fixed location with respect to the incident beam and the crystal is rotated on a spindle so that as Laue conditions are met, spots are produced on the detector at the diffraction angle

Multiple scattering



If more than one reciprocal lattice point is on the Ewald sphere, scattering can occur internal to the crystal.

Multiple scattering



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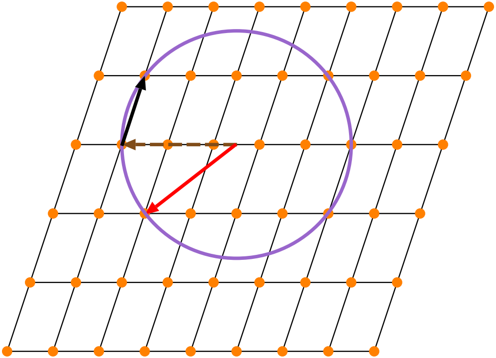
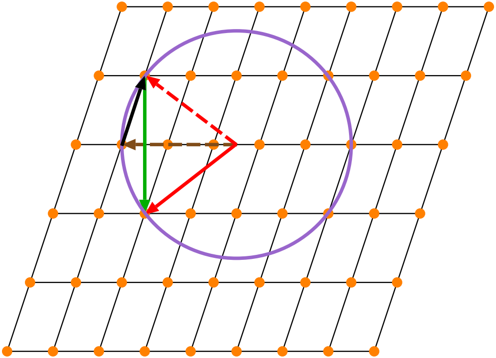
The xrays are first scattered along $\vec{k}_{int}$



If more than one reciprocal lattice point is on the Ewald sphere, scattering can occur internal to the crystal.

The xrays are first scattered along $\vec{k}_{int}$ then along the reciprocal lattice vector which connects the two points on the Ewald sphere, $\vec{G}$

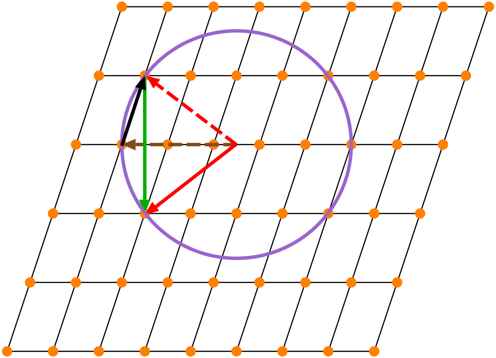
Multiple scattering



If more than one reciprocal lattice point is on the Ewald sphere, scattering can occur internal to the crystal.

The xrays are first scattered along $\vec{k}_{int}$ then along the reciprocal lattice vector which connects the two points on the Ewald sphere, $\vec{G}$ and to the detector at $\vec{k}'$.

Multiple scattering



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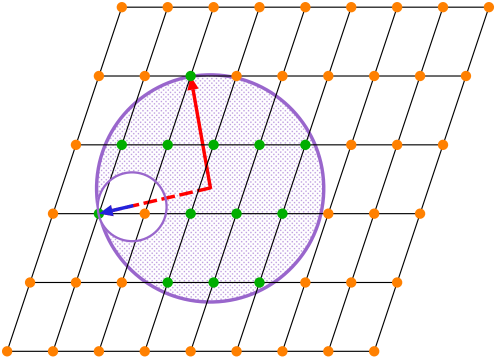
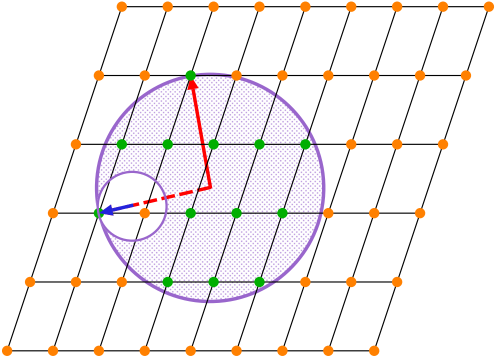
This is the cause of monochromator glitches which sometimes remove intensity but can also add intensity to the reflection the detector is set to measure.

Laue diffraction



The Laue diffraction technique uses a wide range of radiation from $\vec{k}_{min}$ to $\vec{k}_{max}$

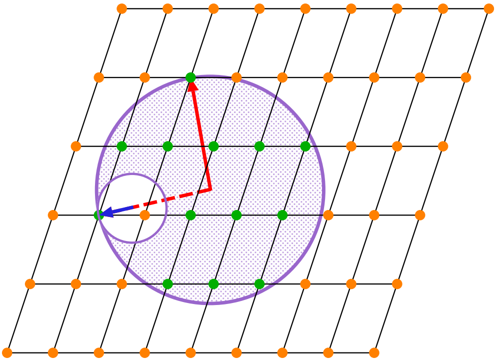
Laue diffraction



The Laue diffraction technique uses a wide range of radiation from $\vec{k}_{min}$ to $\vec{k}_{max}$

These define two Ewald spheres and a volume between them such that any reciprocal lattice point which lies in the volume will meet the Laue condition for reflection.

Laue diffraction

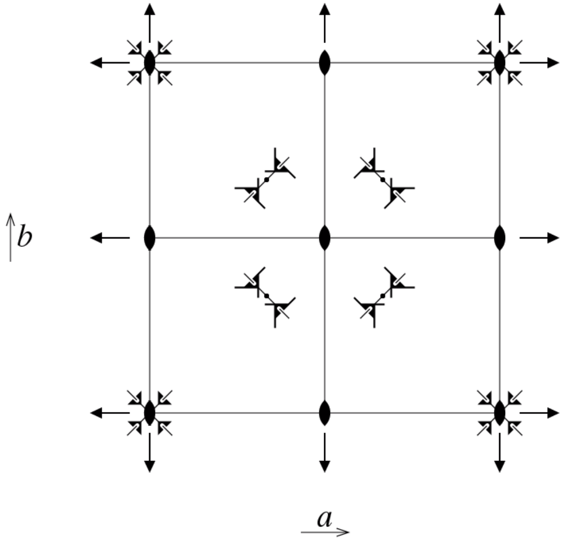


The Laue diffraction technique uses a wide range of radiation from $\vec{k}_{min}$ to $\vec{k}_{max}$

These define two Ewald spheres and a volume between them such that any reciprocal lattice point which lies in the volume will meet the Laue condition for reflection.

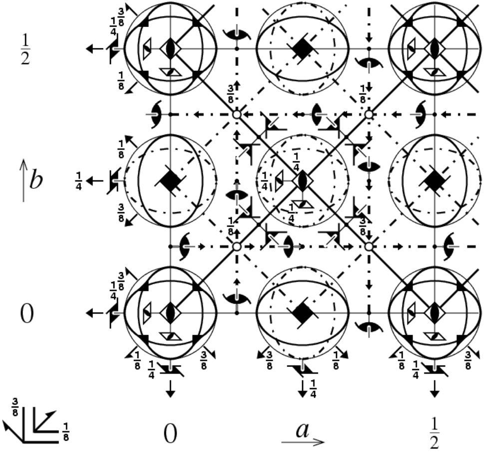
This technique is useful for taking data on crystals which are changing or may degrade in the beam with a single shot of x-rays on a 2D detector.

*P*23 *P* 2 3 23 No. 195



1 x, y, z
2 $x, \bar{y}, \bar{z}$
3 $\bar{x}, y, \bar{z}$
4 $\bar{x}, \bar{y}, z$
5 z, x, y
6 $\bar{z}, \bar{x}, y$
7 $z, \bar{x}, \bar{y}$
8 $\bar{z}, x, \bar{y}$
9 y, z, x
10 $\bar{y}, z, \bar{x}$
11 $\bar{y}, \bar{z}, x$
12 $y, \bar{z}, \bar{x}$

$Fd\bar{3}m$ $F\,4_1/d\,\bar{3}\,2/m$ $m\bar{3}m$ No. 227



1	x, y, z	25	$\frac{1}{4}-x, \frac{1}{4}-y, \frac{1}{4}-z$
2	$x, \bar{y}, \bar{z}$	26	$\frac{1}{4}-x, \frac{1}{4}+y, \frac{1}{4}+z$
3	$\bar{x}, y, \bar{z}$	27	$\frac{1}{4}+x, \frac{1}{4}-y, \frac{1}{4}+z$
4	$\bar{x}, \bar{y}, z$	28	$\frac{1}{4}+x, \frac{1}{4}+y, \frac{1}{4}-z$
5	z, x, y	29	$\frac{1}{4}-z, \frac{1}{4}-x, \frac{1}{4}-y$
6	$\bar{z}, \bar{x}, y$	30	$\frac{1}{4}+z, \frac{1}{4}+x, \frac{1}{4}-y$
7	$z, \bar{x}, \bar{y}$	31	$\frac{1}{4}-z, \frac{1}{4}+x, \frac{1}{4}+y$
8	$\bar{z}, x, \bar{y}$	32	$\frac{1}{4}+z, \frac{1}{4}-x, \frac{1}{4}+y$
9	y, z, x	33	$\frac{1}{4}-y, \frac{1}{4}-z, \frac{1}{4}-x$
10	$\bar{y}, z, \bar{x}$	34	$\frac{1}{4}+y, \frac{1}{4}-z, \frac{1}{4}+x$
11	$\bar{y}, \bar{z}, x$	35	$\frac{1}{4}+y, \frac{1}{4}+z, \frac{1}{4}-x$
12	$y, \bar{z}, \bar{x}$	36	$\frac{1}{4}-y, \frac{1}{4}+z, \frac{1}{4}+x$
13	$\frac{1}{4}+x, \frac{1}{4}-z, \frac{1}{4}+y$	37	$\bar{x}, z, \bar{y}$
14	$\frac{1}{4}+x, \frac{1}{4}+z, \frac{1}{4}-y$	38	$\bar{x}, \bar{z}, y$
15	$\frac{1}{4}-x, \frac{1}{4}-z, \frac{1}{4}-y$	39	x, z, y
16	$\frac{1}{4}-x, \frac{1}{4}+z, \frac{1}{4}+y$	40	$x, \bar{z}, \bar{y}$
17	$\frac{1}{4}+z, \frac{1}{4}+y, \frac{1}{4}-x$	41	$\bar{z}, \bar{y}, x$
18	$\frac{1}{4}-z, \frac{1}{4}+y, \frac{1}{4}+x$	42	$z, \bar{y}, \bar{x}$
19	$\frac{1}{4}-z, \frac{1}{4}-y, \frac{1}{4}-x$	43	z, y, x
20	$\frac{1}{4}+z, \frac{1}{4}-y, \frac{1}{4}+x$	44	$\bar{z}, y, \bar{x}$
21	$\frac{1}{4}-y, \frac{1}{4}+x, \frac{1}{4}+z$	45	$y, \bar{x}, \bar{z}$
22	$\frac{1}{4}+y, \frac{1}{4}-x, \frac{1}{4}+z$	46	$\bar{y}, x, \bar{z}$
23	$\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$	47	y, x, z
24	$\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}-z$	48	$\bar{y}, \bar{x}, z$

$+ (0,\frac{1}{2},\frac{1}{2}), (\frac{1}{2},0,\frac{1}{2}), (\frac{1}{2},\frac{1}{2},0)$

Wyckoff Positions of Group 195 (*P*23)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
12	j	1	(x,y,z) (-x,-y,z) (-x,y,-z) (x,-y,-z) (z,x,y) (z,-x,-y) (-z,-x,y) (-z,x,-y) (y,z,x) (-y,z,-x) (y,-z,-x) (-y,-z,x)
6	i	2..	(x,1/2,1/2) (-x,1/2,1/2) (1/2,x,1/2) (1/2,-x,1/2) (1/2,1/2,x) (1/2,1/2,-x)
6	h	2..	(x,1/2,0) (-x,1/2,0) (0,x,1/2) (0,-x,1/2) (1/2,0,x) (1/2,0,-x)
6	g	2..	(x,0,1/2) (-x,0,1/2) (1/2,x,0) (1/2,-x,0) (0,1/2,x) (0,1/2,-x)
6	f	2..	(x,0,0) (-x,0,0) (0,x,0) (0,-x,0) (0,0,x) (0,0,-x)
4	e	.3.	(x,x,x) (-x,-x,x) (-x,x,-x) (x,-x,-x)
3	d	222 . .	(1/2,0,0) (0,1/2,0) (0,0,1/2)
3	c	222 . .	(0,1/2,1/2) (1/2,0,1/2) (1/2,1/2,0)
1	b	23.	(1/2,1/2,1/2)
1	a	23.	(0,0,0)

Wyckoff Positions of Group 227 (*Fd*-3*m*) [origin choice 1]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
			(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
192	i	1	(x,y,z) (-x,-y+1/2,z+1/2) (-x+1/2,y+1/2,-z) (x+1/2,-y,-z+1/2) (z,x,y) (z+1/2,-x,-y+1/2) (-z,-x+1/2,y+1/2) (-z+1/2,x+1/2,-y) (y,z,x) (-y+1/2,z+1/2,-x) (y+1/2,-z,-x+1/2) (-y,-z+1/2,x+1/2) (y+3/4,x+1/4,-z+3/4) (-y+1/4,-x+1/4,-z+1/4) (y+1/4,-x+3/4,z+3/4) (-y+3/4,x+3/4,z+1/4) (x+3/4,z+1/4,-y+3/4) (-x+3/4,z+3/4,y+1/4) (-x+1/4,-z+1/4,-y+1/4) (x+1/4,-z+3/4,y+3/4) (z+3/4,y+1/4,-x+3/4) (z+1/4,-y+3/4,x+3/4) (-z+3/4,y+3/4,x+1/4) (-z+1/4,-y+1/4,-x+1/4) (-x+1/4,-y+1/4,-z+1/4) (x+1/4,y+3/4,-z+3/4) (x+3/4,-y+3/4,z+1/4) (-x+3/4,y+1/4,z+3/4) (-z+1/4,-x+1/4,-y+1/4) (-z+3/4,x+1/4,y+3/4) (z+1/4,x+3/4,-y+3/4) (z+3/4,-x+3/4,y+1/4) (-y+1/4,-z+1/4,-x+1/4) (y+3/4,-z+3/4,x+1/4) (-y+3/4,z+1/4,x+3/4) (y+1/4,z+3/4,-x+3/4) (-y+1/2,-x,z+1/2) (y,x,z) (-y,x+1/2,-z+1/2) (y+1/2,-x+1/2,-z) (-x+1/2,-z,y+1/2) (x+1/2,-z+1/2,-y) (x,z,y) (-x,z+1/2,-y+1/2) (-z+1/2,-y,x+1/2) (-z,y+1/2,-x+1/2) (z+1/2,-y+1/2,-x) (z,y,x)
96	h	..2	(1/8,y,-y+1/4) (7/8,-y+1/2,-y+3/4) (3/8,y+1/2,y+3/4) (5/8,-y,y+1/4) (-y+1/4,1/8,y) (-y+3/4,7/8,-y+1/2) (y+3/4,3/8,y+1/2) (y+1/4,5/8,-y) (y,-y+1/4,1/8) (-y+1/2,-y+3/4,7/8) (y+1/2,y+3/4,3/8) (-y,y+1/4,5/8) (1/8,-y+1/4,y) (3/8,y+3/4,y+1/2) (7/8,-y+3/4,-y+1/2) (5/8,y+1/4,-y) (y,1/8,-y+1/4) (y+1/2,3/8,y+3/4) (-y+1/2,7/8,-y+3/4) (-y,5/8,y+1/4) (-y+1/4,y,1/8) (y+3/4,y+1/2,3/8) (-y+3/4,-y+1/2,7/8) (y+1/4,-y,5/8)
96	g	..m	(x,x,z) (-x,-x+1/2,z+1/2) (-x+1/2,x+1/2,-z) (x+1/2,-x,-z+1/2) (z,x,x) (z+1/2,-x,-x+1/2) (-z,-x+1/2,x+1/2) (-z+1/2,x+1/2,-x) (x,z,x) (-x+1/2,z+1/2,-x) (x+1/2,-z,-x+1/2) (-x,-z+1/2,x+1/2) (x+3/4,x+1/4,-z+3/4) (-x+1/4,-x+1/4,-z+1/4) (x+1/4,-x+3/4,z+3/4) (-x+3/4,x+3/4,z+1/4) (x+3/4,z+1/4,-x+3/4) (-x+3/4,z+3/4,x+1/4) (-x+1/4,-z+1/4,-x+1/4) (x+1/4,-z+3/4,x+3/4) (z+3/4,x+1/4,-x+3/4) (z+1/4,-x+3/4,x+3/4) (-z+3/4,x+3/4,x+1/4) (-z+1/4,-x+1/4,-x+1/4)
48	f	2.m m	(x,0,0) (-x,1/2,1/2) (0,x,0) (1/2,-x,1/2) (0,0,x) (1/2,1/2,-x) (3/4,x+1/4,3/4) (1/4,-x+1/4,1/4) (x+3/4,1/4,3/4) (-x+3/4,3/4,1/4) (3/4,1/4,-x+3/4) (1/4,3/4,x+3/4)
32	e	.3m	(x,x,x) (-x,-x+1/2,x+1/2) (-x+1/2,x+1/2,-x) (x+1/2,-x,-x+1/2) (x+3/4,x+1/4,-x+3/4) (-x+1/4,-x+1/4,-x+1/4) (x+1/4,-x+3/4,x+3/4) (-x+3/4,x+3/4,x+1/4)
16	d	.-3m	(5/8,5/8,5/8) (3/8,7/8,1/8) (7/8,1/8,3/8) (1/8,3/8,7/8)
16	c	.-3m	(1/8,1/8,1/8) (7/8,3/8,5/8) (3/8,5/8,7/8) (5/8,7/8,3/8)
8	b	-43m	(1/2,1/2,1/2) (1/4,3/4,1/4)
8	a	-43m	(0,0,0) (3/4,1/4,3/4)

Diffraction from a Truncated Surface

For an infinite sample, the diffraction spots are infinitesimally sharp.

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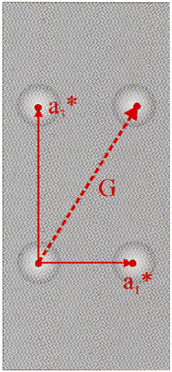

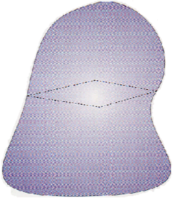

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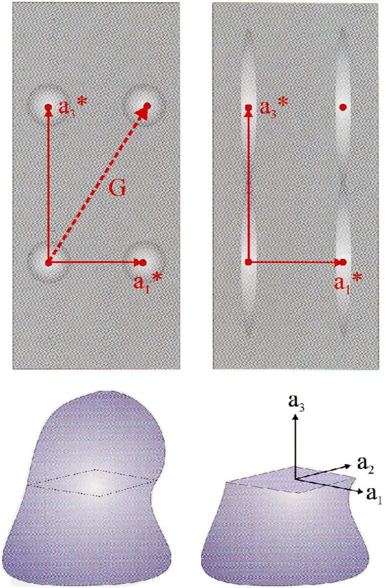

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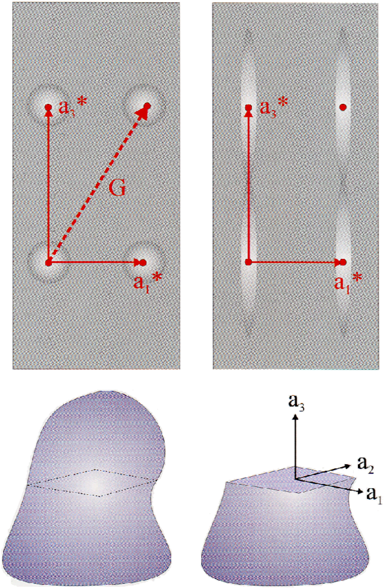

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The scattering intensity can be obtained by treating the charge distribution as a convolution of an infinite sample with a step function in the z-direction.

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When l is an integer (meeting the Laue condition), the scattering factor is infinite but just off this value, the scattering factor can be computed by letting $Q_z = q_z + 2\pi/a_3$, with q_z small.

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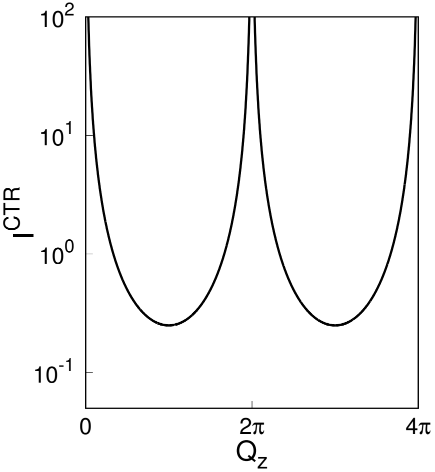
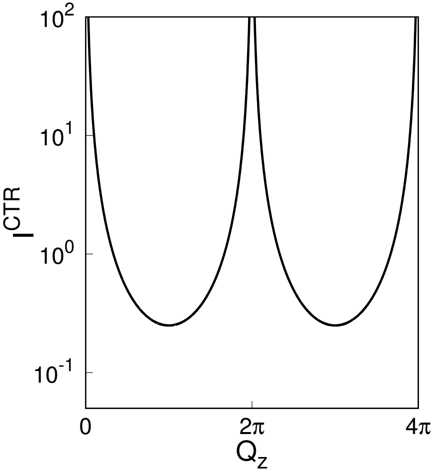


Absorption Effect

Absorption effects can be included as well by adding a term for each layer penetrated



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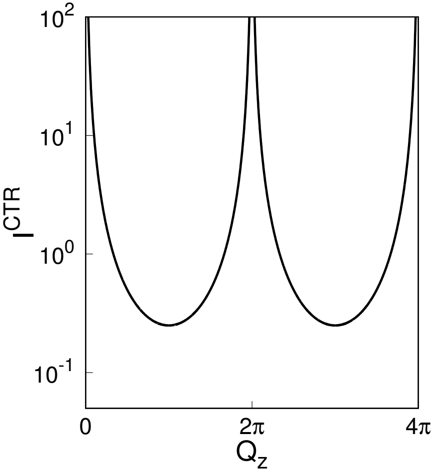

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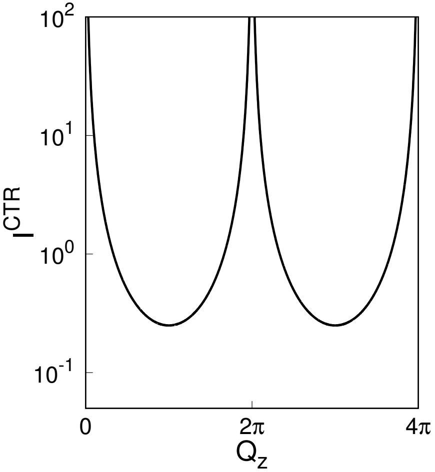

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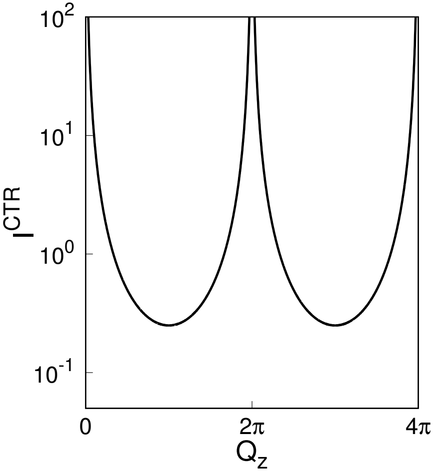

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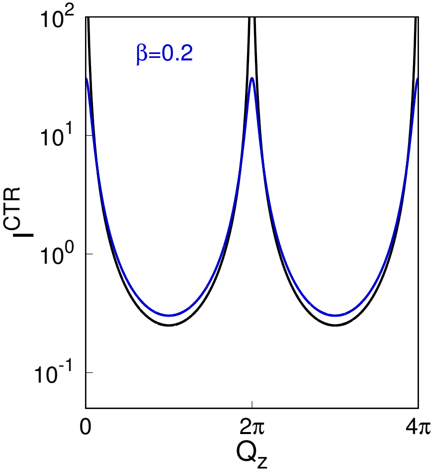

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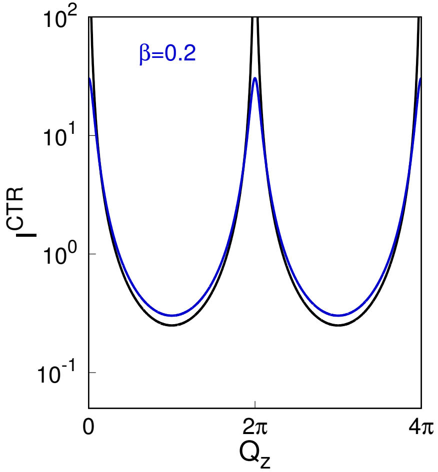
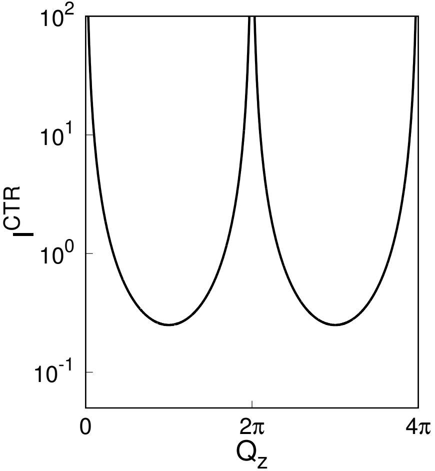
This removes the infinity and increases the scattering profile of the crystal truncation rod



Density Effect

The CTR profile is sensitive to the termination of the surface. This makes it an ideal probe of electron density of adsorbed species or single atom overlayers.



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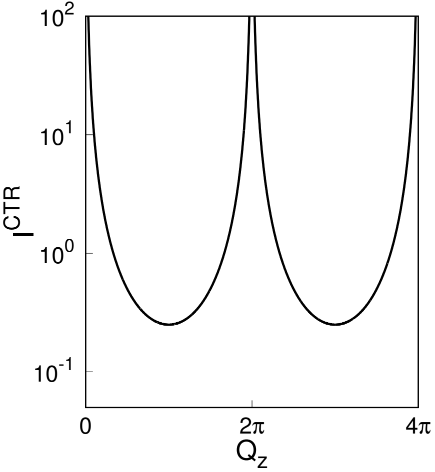

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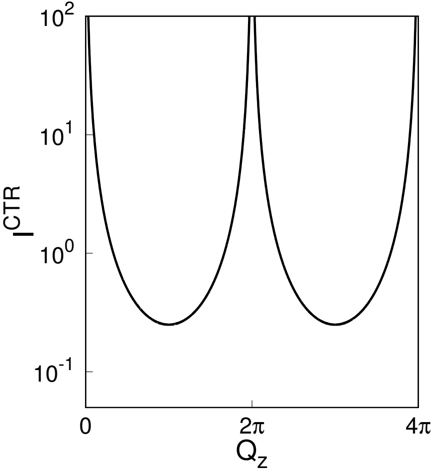

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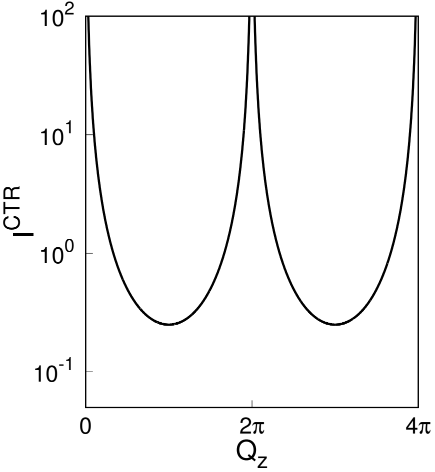

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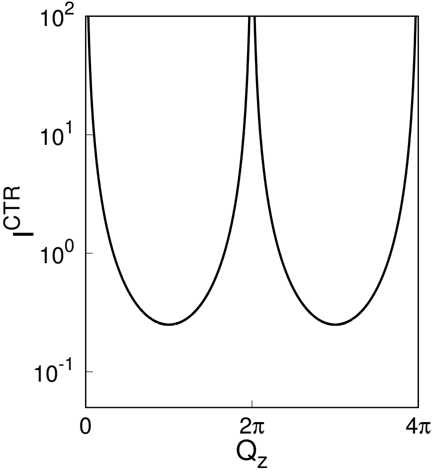

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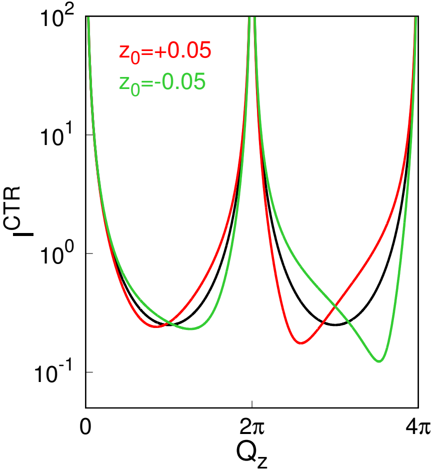

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This effect gets larger for larger momentum transfers