Today's Outline - February 27, 2020

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- Lattices & space groups

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Reading assignment: Chapter 5.2

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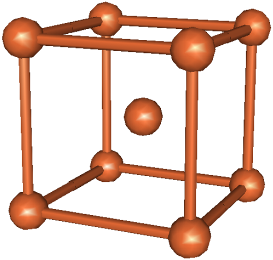
Reading assignment: Chapter 5.2

Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Tuesday, March 10, 2020

BCC structure factor

In the body centered cubic structure, there are 2 atoms in the conventional, cubic unit cell. These are located at



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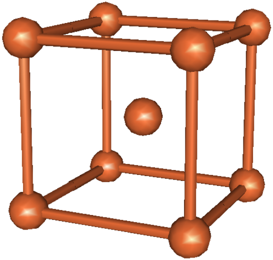

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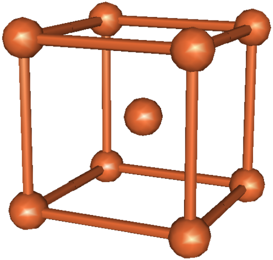

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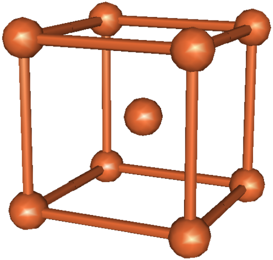

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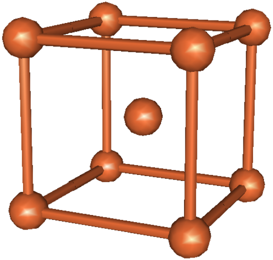

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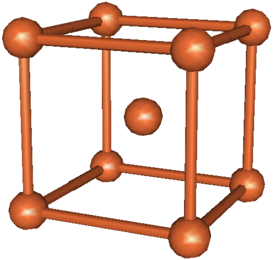

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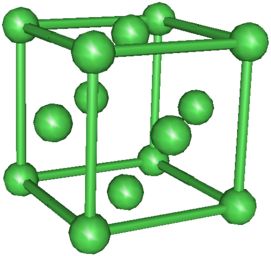

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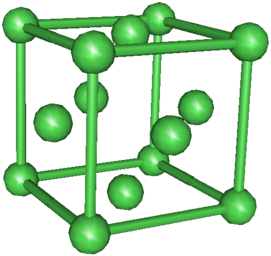

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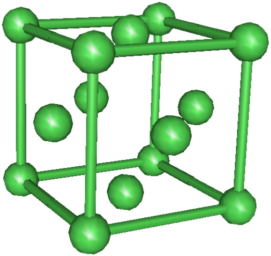

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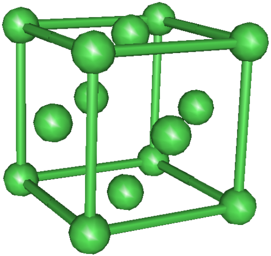

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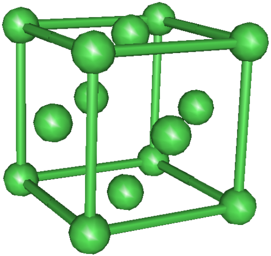

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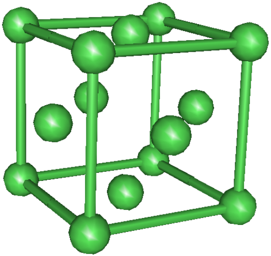

Diamond structure

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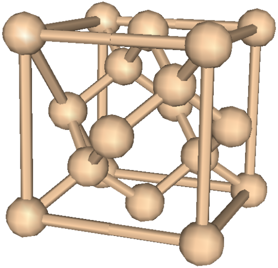

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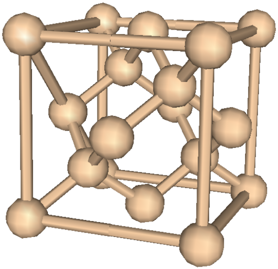

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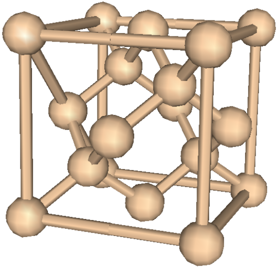
$$F_{hkl}^{diamond} = f(\vec{G})\Big(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k+l)/2} + e^{i\pi(3h+3k+l)/2} + e^{i\pi(h+3k+3l)/2} + e^{i\pi(3h+k+3l)/2}\Big)$$



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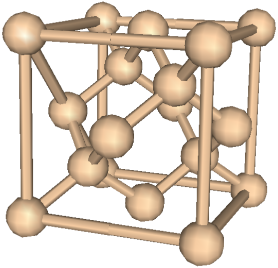
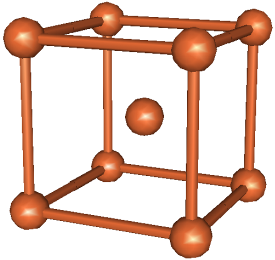


This is non-zero when h,k,l all even and $h+k+l=4n$ or h,k,l all odd

Heteroatomic structures



← bcc

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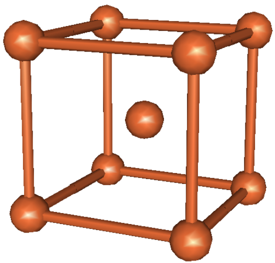

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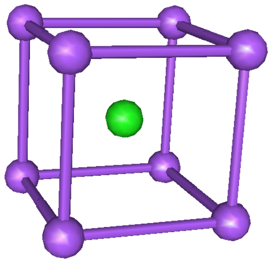
sc →



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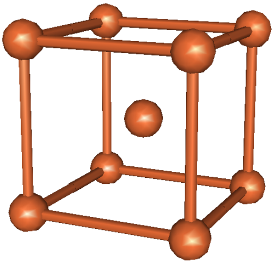

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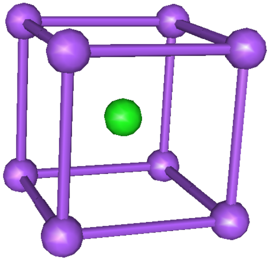

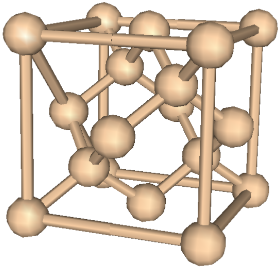

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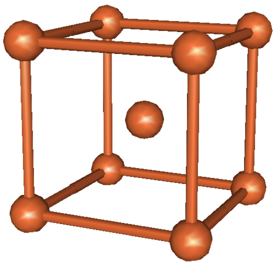

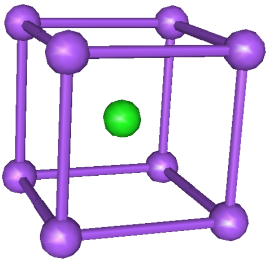

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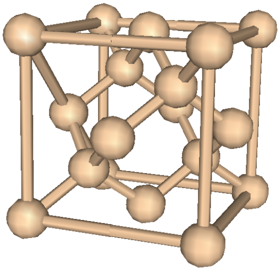

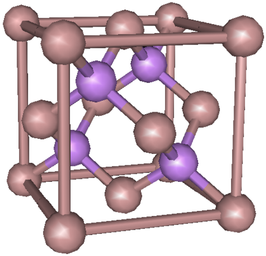

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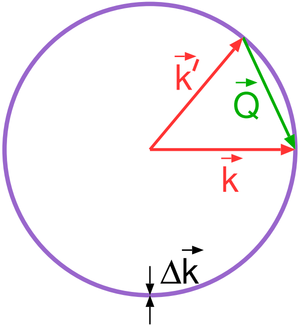
The sphere radius is set by the length of the $\vec{k}$ and $\vec{k}'$ vectors which characterize the incident and scattered (where the detector is placed) x-rays and $\Delta\vec{k}$ being the bandwidth of the incident x-rays



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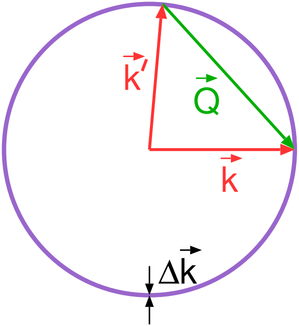

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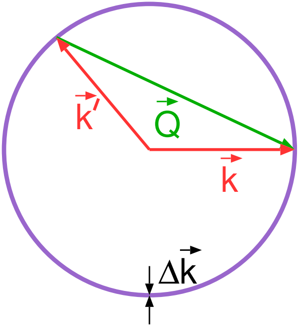

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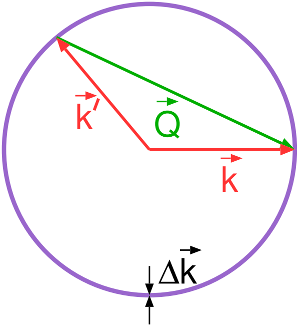

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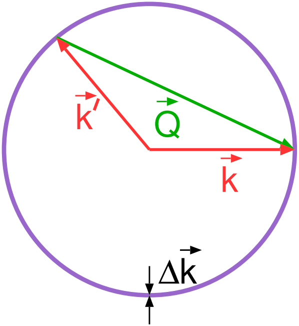

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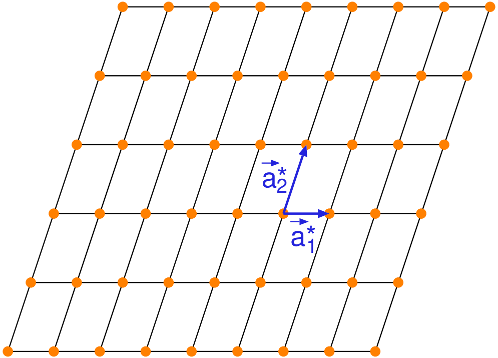
http://www.phillipslab.org/software

Ewald sphere & the reciprocal lattice



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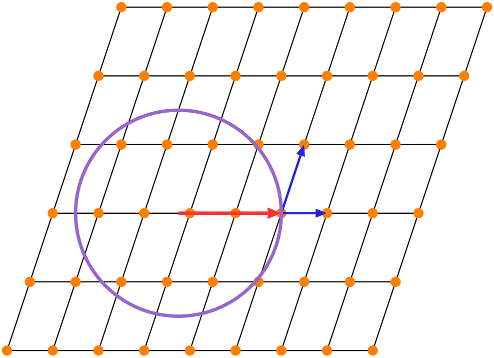
Ewald sphere & the reciprocal lattice



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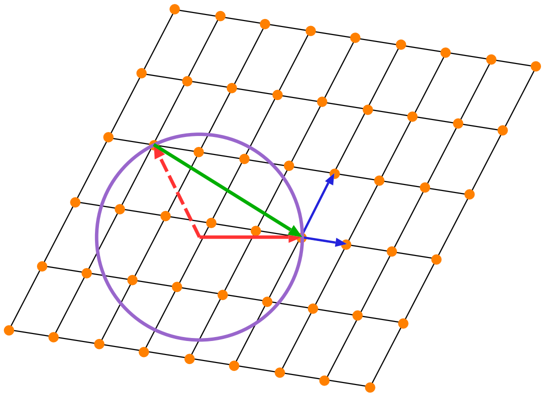

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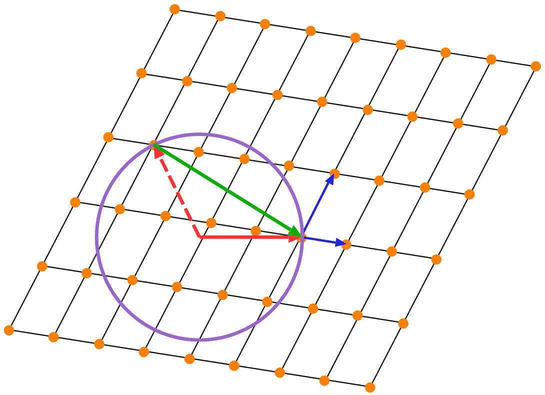

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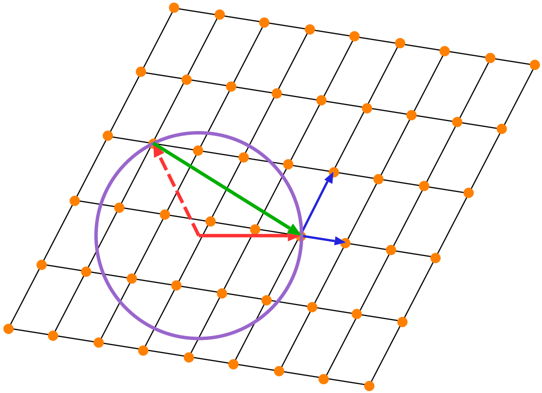

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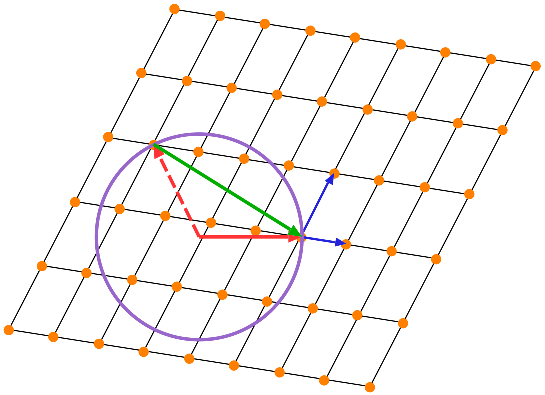
Ewald sphere & the reciprocal lattice



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

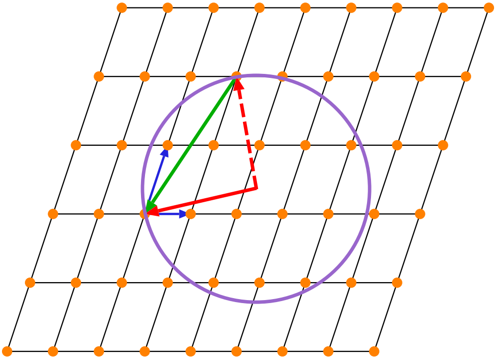
The key parameter is the relative orientation of the incident wave vector $\vec{k}$

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

When the Ewald sphere intersects a reciprocal lattice point there will be a diffraction peak in the direction of the scattered x-rays. The diffraction vector, $\vec{Q}$, is thus a reciprocal lattice vector

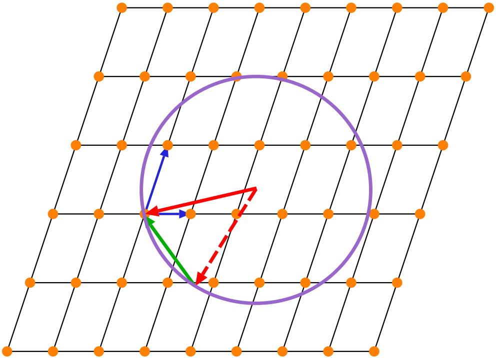
$$\vec{G}_{hlk} = h\vec{a}_1^* + k\vec{a}_2^*$$

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



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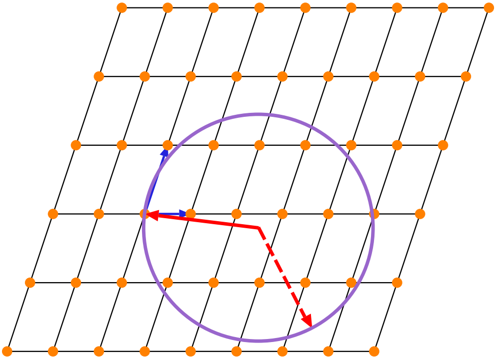
In directions of $\vec{k}'$ (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.

Ewald construction

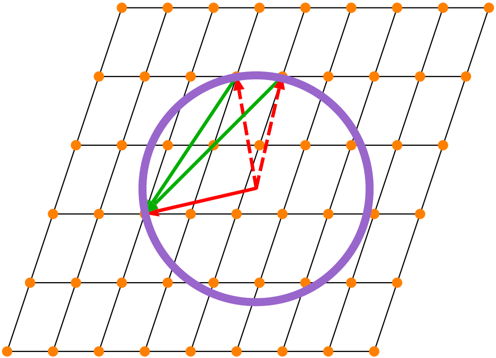


It is often more convenient to visualize the Ewald sphere by keeping the reciprocal lattice fixed and “rotating” the incident beam to visualize the scattering geometry.

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

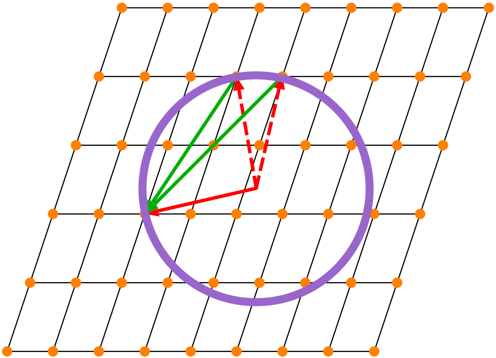
If the crystal is rotated slightly with respect to the incident beam, $\vec{k}$, there may be no Bragg reflections possible at all.

Polychromatic radiation



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

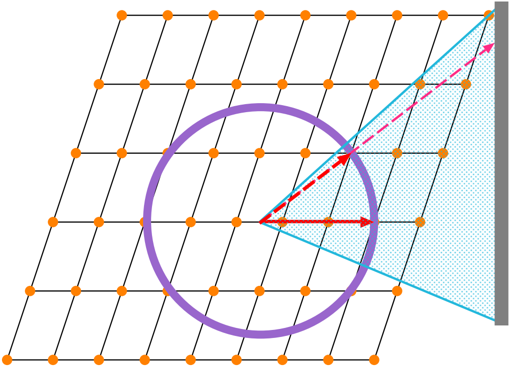
Polychromatic radiation



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

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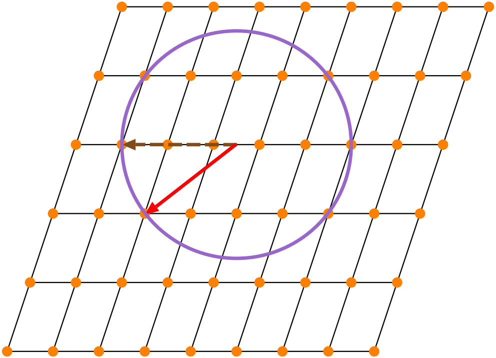
With an area detector, there may then be multiple reflections appearing for a particular orientation (very common with protein crystals where the unit cell is very large).

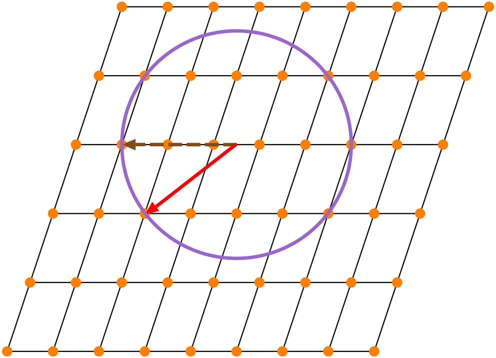
In protein crystallography, the area detector is in a fixed location with respect to the incident beam and the crystal is rotated on a spindle so that as Laue conditions are met, spots are produced on the detector at the diffraction angle

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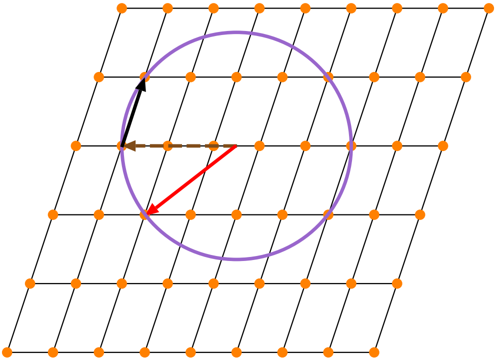
The xrays are first scattered along $\vec{k}_{int}$

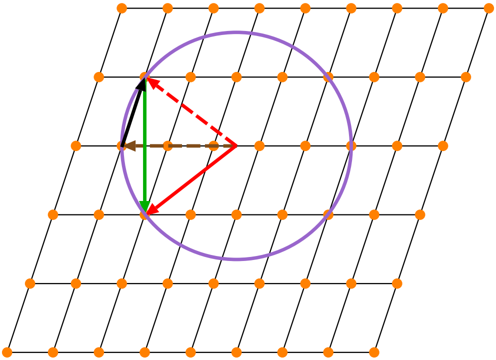
Multiple scattering



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, $\vec{G}$

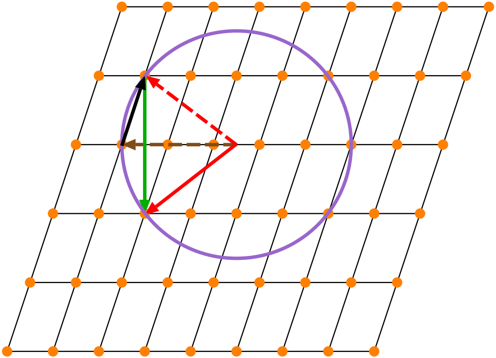
Multiple scattering



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

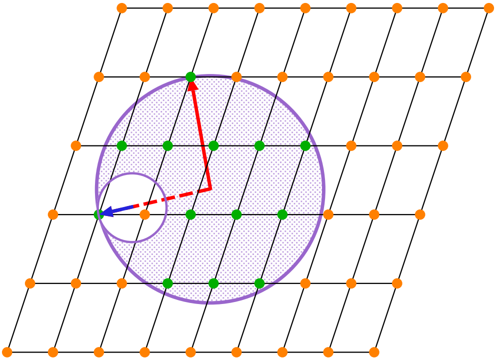


If more than one reciprocal lattice point is on the Ewald sphere, scattering can occur internal to the crystal.

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 $\vec{k}'$.

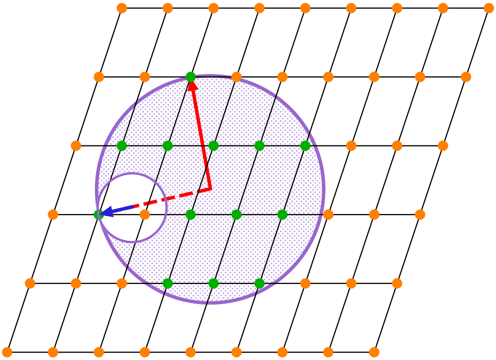
This is the cause of monochromator glitches which sometimes remove intensity but can also add intensity to the reflection the detector is set to measure.

Laue diffraction



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

Laue diffraction



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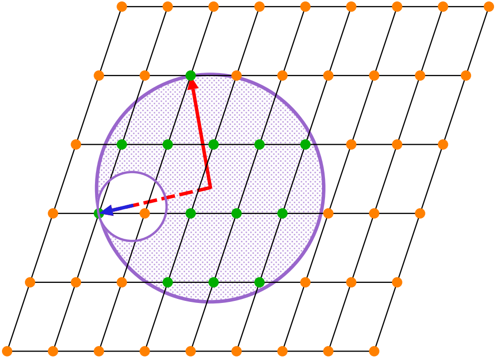
These define two Ewald spheres and a volume between them such that any reciprocal lattice point which lies in the volume will meet the Laue condition for reflection.

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.

Diffraction resources

XRayView

http://www.phillipslab.org/downloads

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GSAS-II

https://subversion.xray.aps.anl.gov/trac/pyGSAS

XRayView demonstration

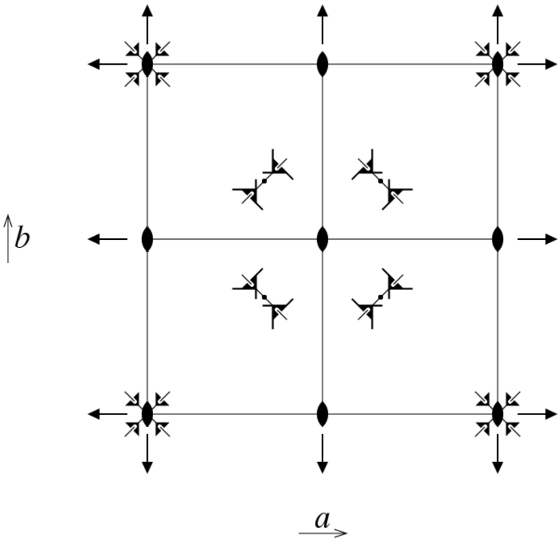
Exercise 1 - Ewald sphere

Exercise 4 - Wavelength

Exercise 8 - Laue diffraction

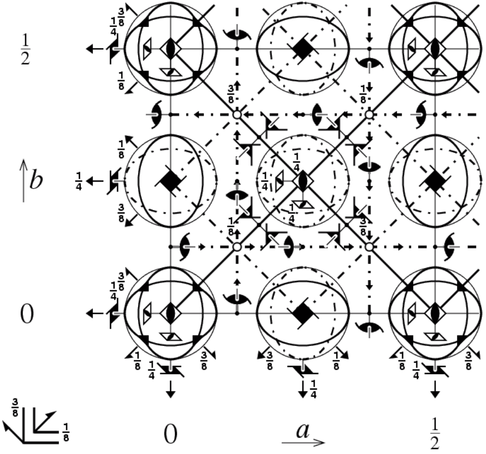
Exercise 9 - Serial crystallography

*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 $y, \bar{z}, \bar{x}$

$Fd\bar{3}m$ $\quad$ $F\,4_1/d\,\bar{3}\,2/m$ $\quad$ $m\bar{3}m$ $\quad$ 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	$\bar{y}, \bar{x}, z$

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

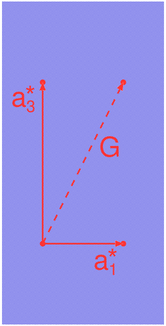
Wyckoff Positions of Group 195 (*P*23)

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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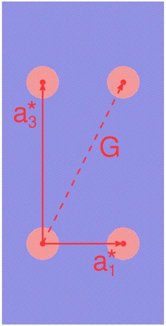

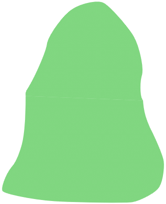

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With finite sample size, these spots grow in extent and become more diffuse.

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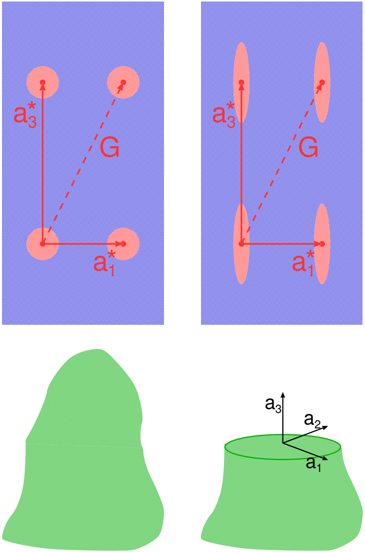

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If the sample is cleaved and left with flat surface, the diffraction will spread into rods perpendicular to the surface.

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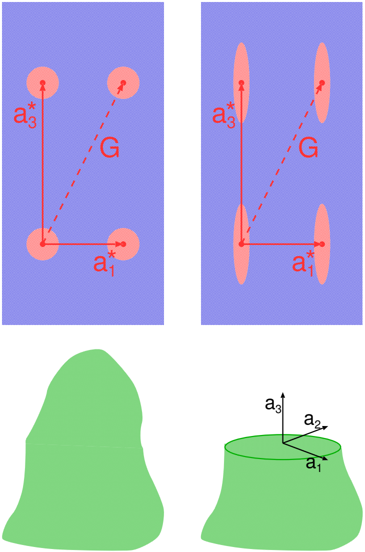

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With finite sample size, these spots grow in extent and become more diffuse.

If the sample is cleaved and left with flat surface, the diffraction will spread into rods perpendicular to the surface.

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.

CTR Scattering Factor

The scattering amplitude F^{CTR} along a crystal truncation rod is given by summing an infinite stack of atomic layers, each with scattering amplitude $A(\vec{Q})$.

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this sum has been discussed previously and gives

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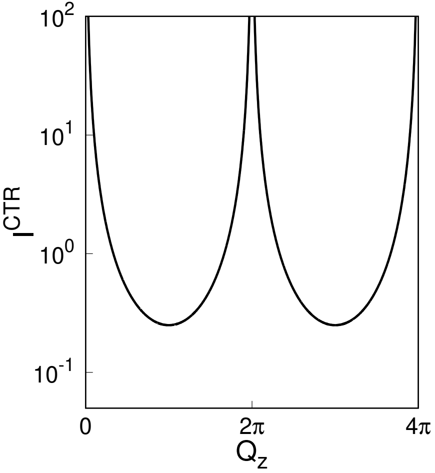

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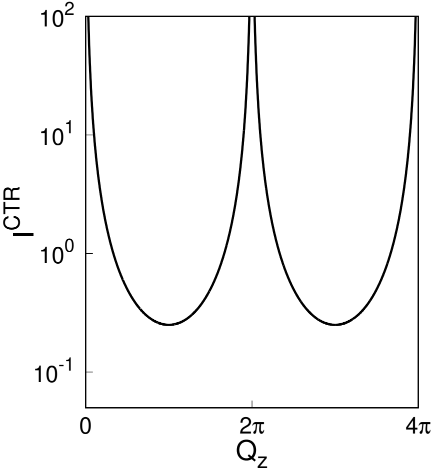
Absorption effects can be included as well by adding a term for each layer penetrated



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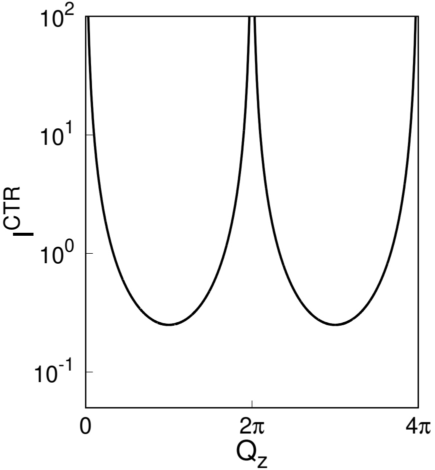

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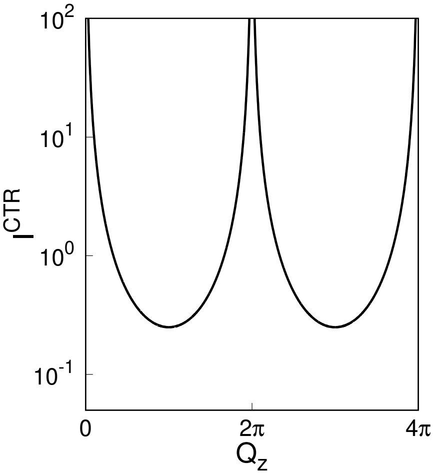

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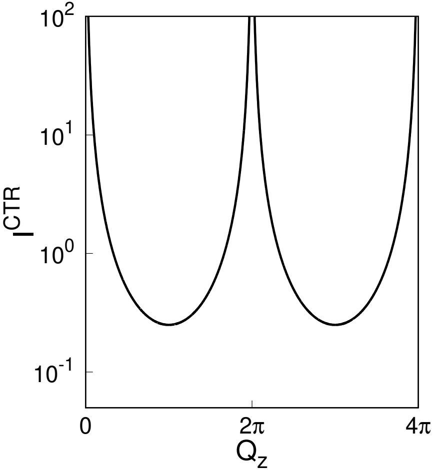

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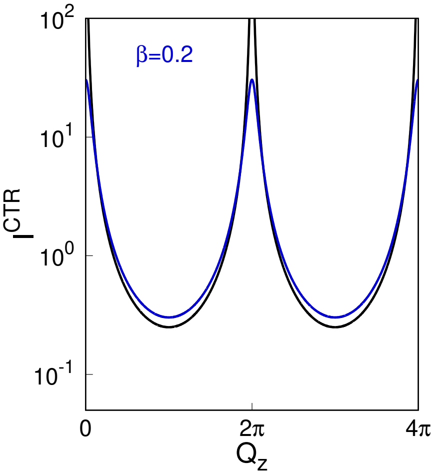

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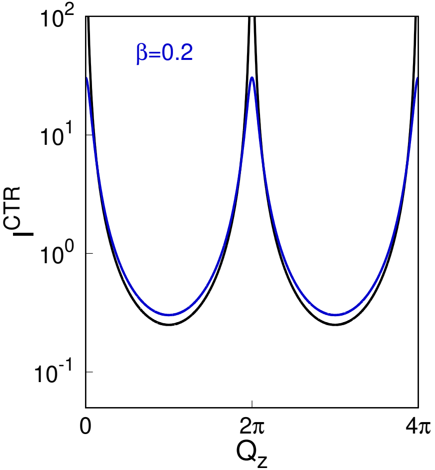
This removes the infinity and increases the scattering profile of the crystal truncation rod



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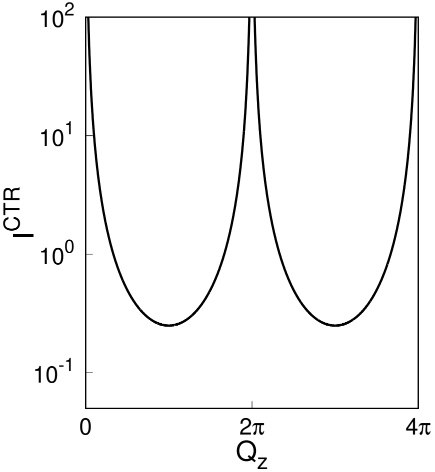
The CTR profile is sensitive to the termination of the surface. This makes it an ideal probe of electron density of adsorbed species or single atom overlayers.



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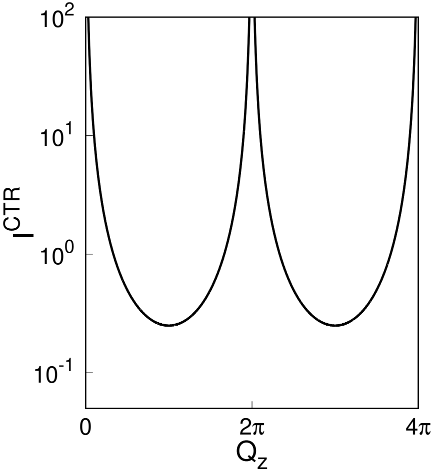

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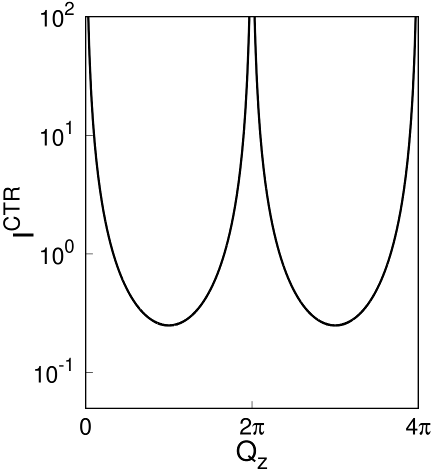

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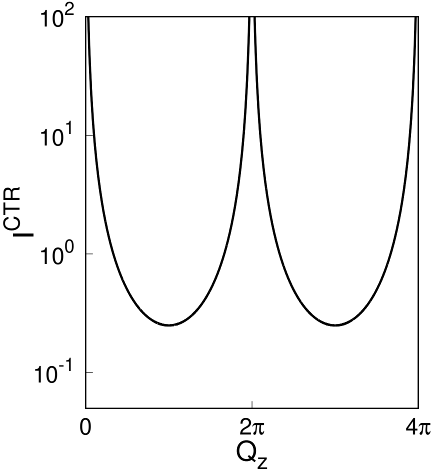

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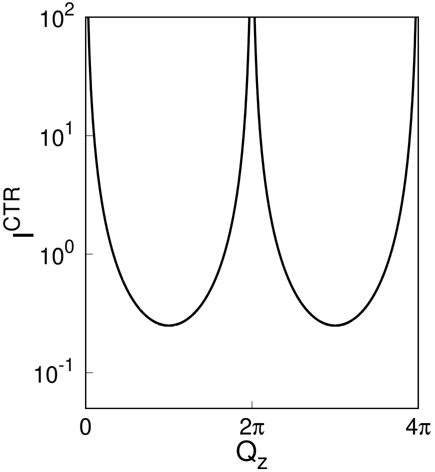

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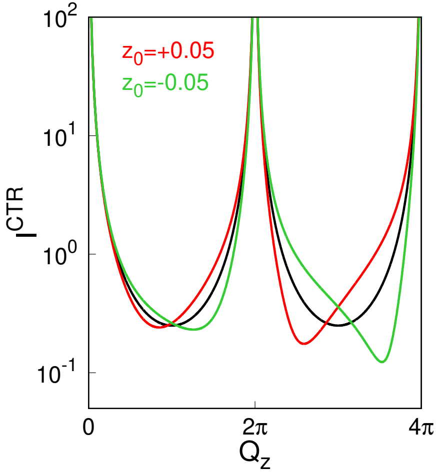

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