Today's outline - October 07, 2021

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- Equivalence of Laue & Bragg conditions

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Reading Assignment: Chapter 5.4

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- Equivalence of Laue & Bragg conditions
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Reading Assignment: Chapter 5.4

Homework Assignment #04:
Chapter 4: 2,4,6,7.10
due Tuesday, October 19, 2021

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- Equivalence of Laue & Bragg conditions
- Crystal structure factor
- Lattices & space groups
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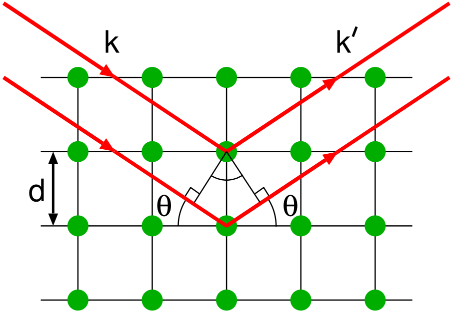
Reading Assignment: Chapter 5.4

Homework Assignment #04:
Chapter 4: 2,4,6,7.10
due Tuesday, October 19, 2021

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

Bragg condition



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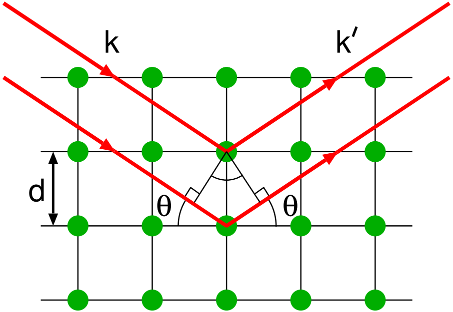
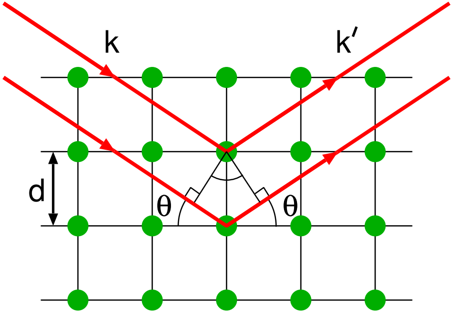


The Bragg condition for diffraction is derived by assuming specular reflection from parallel planes separated by a distance d.

Bragg condition



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The ray reflecting from the deeper plane travels an extra distance $2d\sin\theta$

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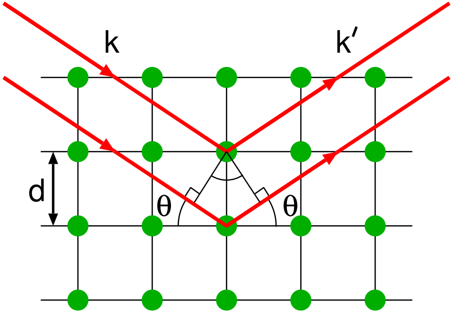

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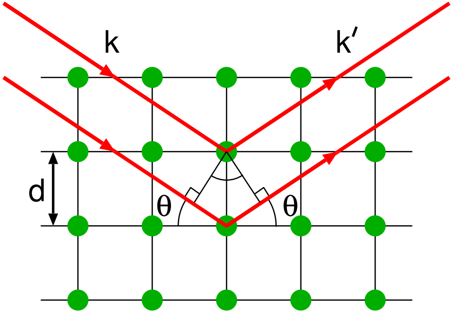

$$2d \sin\theta = \lambda$$

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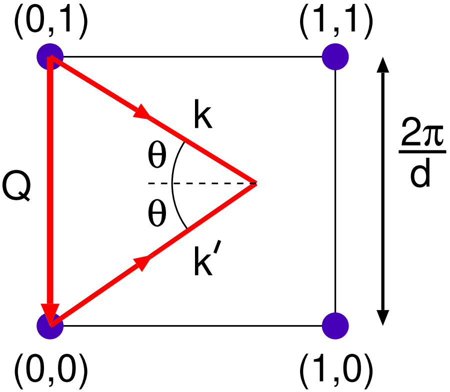
Laue condition

The Laue condition states that the scattering vector must be equal to a reciprocal lattice vector



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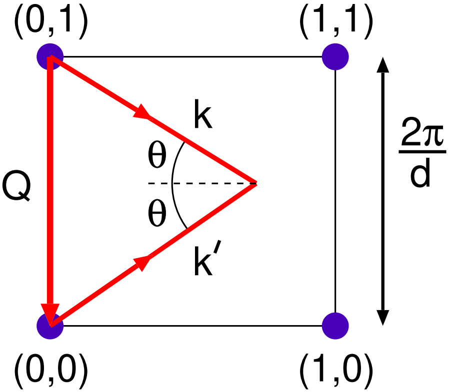

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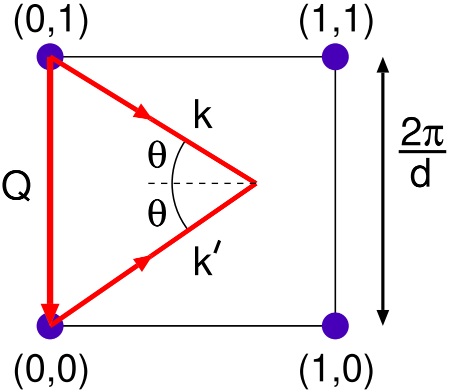
$$\vec{Q} = \vec{G_{hk}}$$



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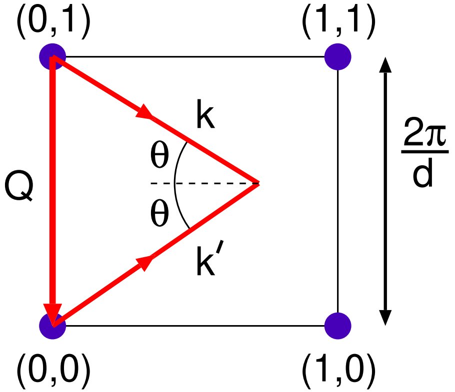

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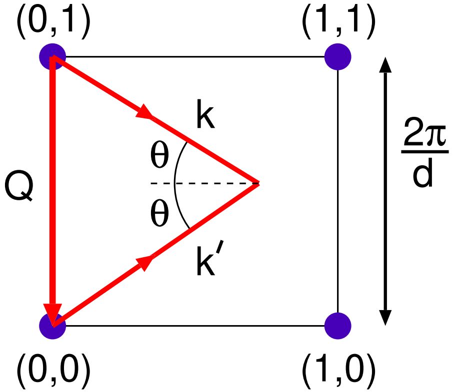

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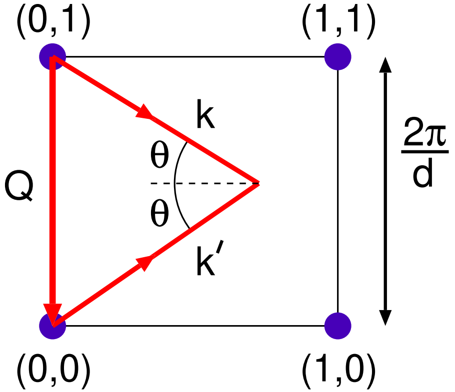

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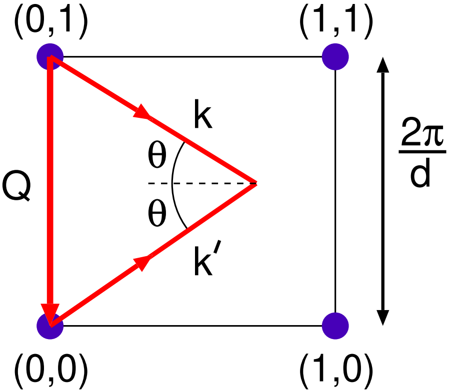

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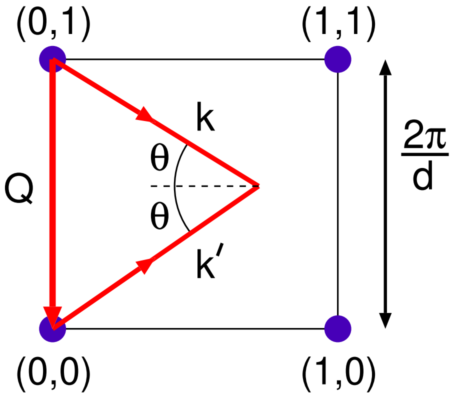
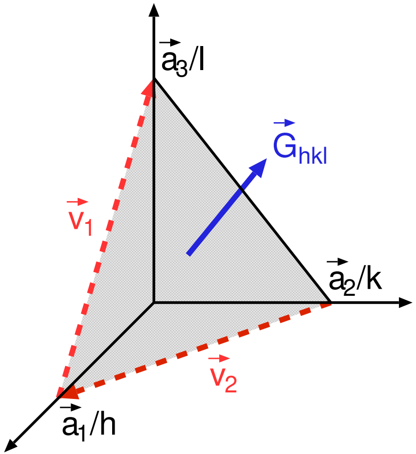
Thus the Bragg and Laue conditions are equivalent



General proof of Bragg-Laue equivalence



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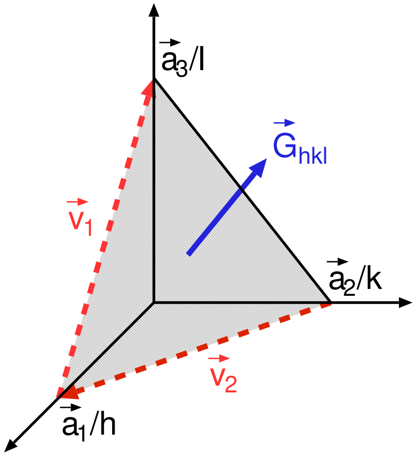
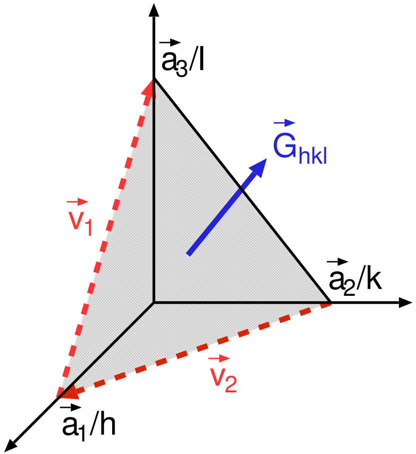


Must show that for each point in reciprocal space, there exists a set of planes in the real space lattice such that:

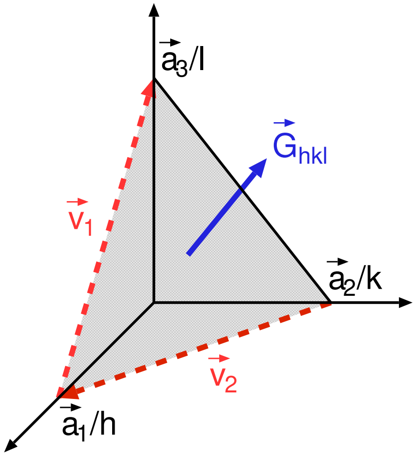
General proof of Bragg-Laue equivalence



Must show that for each point in reciprocal space, there exists a set of planes in the real space lattice such that:

$\vec{G}_{hkl}$ is perpendicular to the planes with Miller indices (hkl)

General proof of Bragg-Laue equivalence



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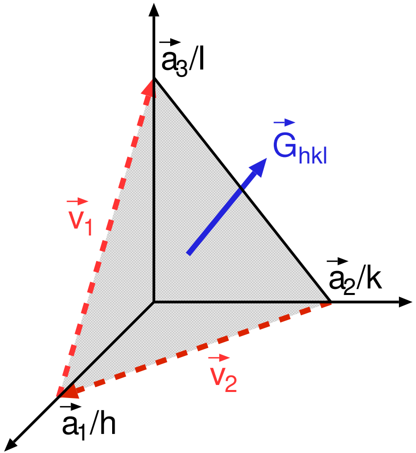
$$|\vec{G}_{hkl}| = \frac{2\pi}{d_{hkl}}$$

General proof of Bragg-Laue equivalence



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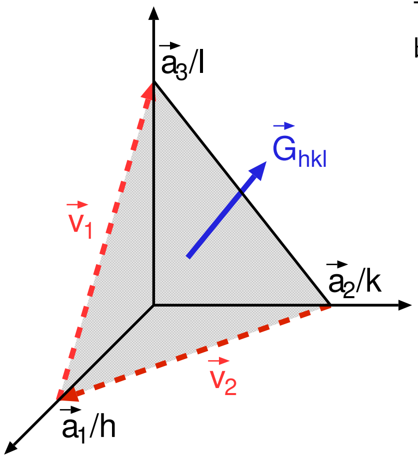
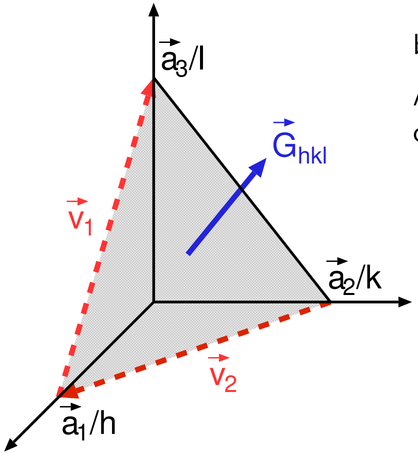


The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

General proof of Bragg-Laue equivalence



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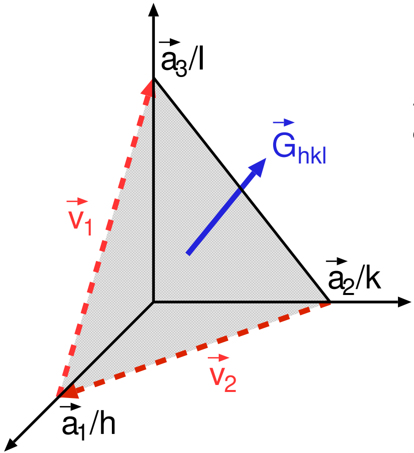

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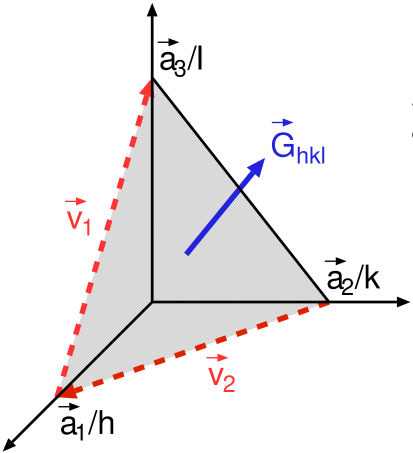

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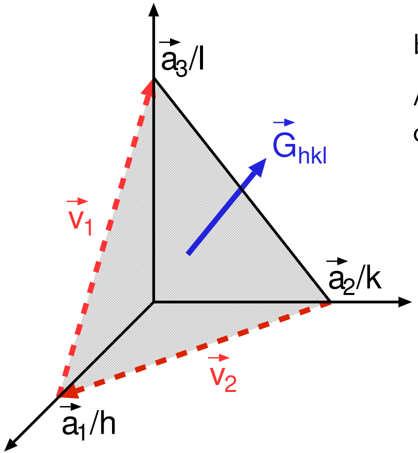

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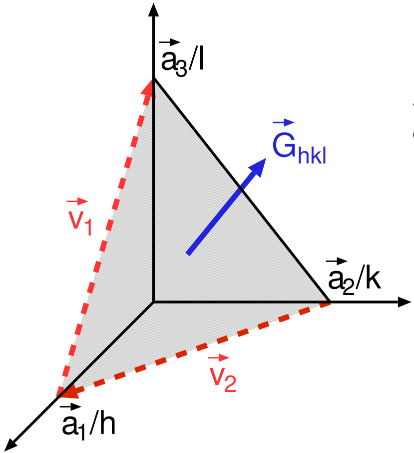

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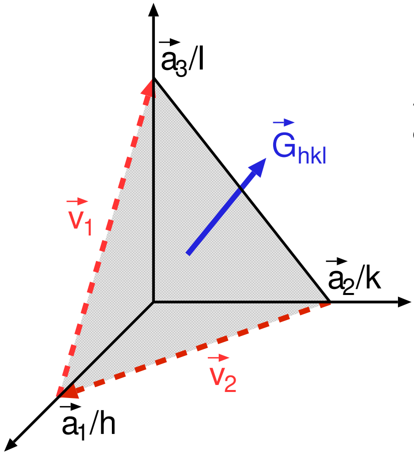
$$\vec{G}_{hkl} \cdot \vec{v} = (h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*) \cdot \left((\epsilon_2 - \epsilon_1)\frac{\vec{a}_1}{h} - \epsilon_2 \frac{\vec{a}_2}{k} + \epsilon_1 \frac{\vec{a}_3}{l} \right)$$

General proof of Bragg-Laue equivalence



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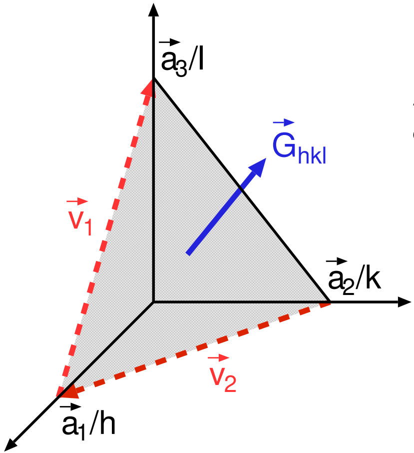
General proof of Bragg-Laue equivalence



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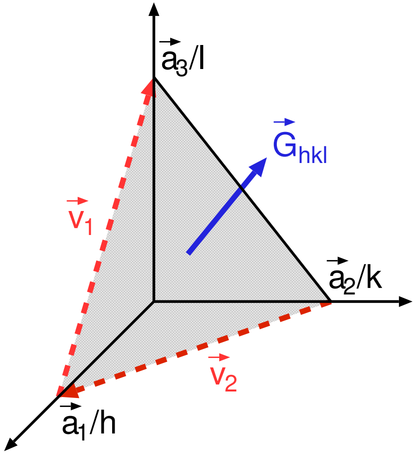
Thus $\vec{G}_{hkl}$ is indeed normal to the plane with Miller indices (hkl)

General proof of Bragg-Laue equivalence



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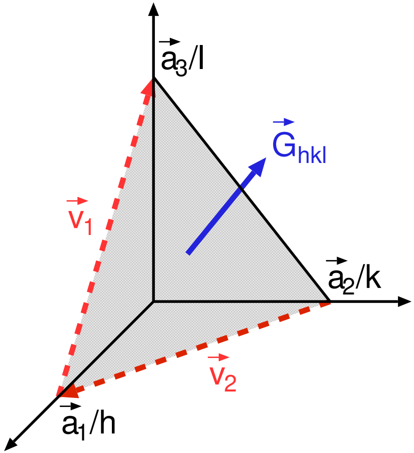
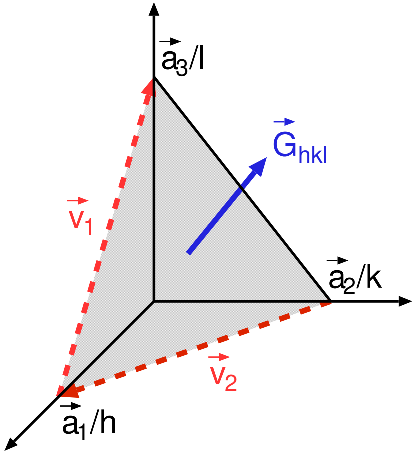


The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

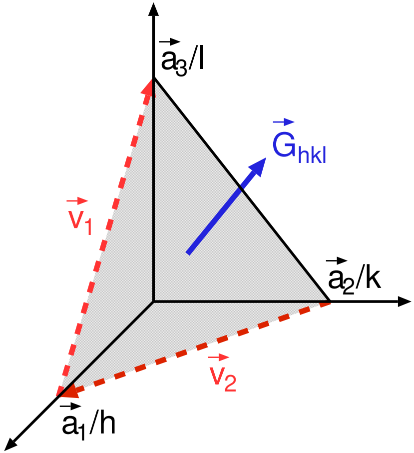
General proof of Bragg-Laue equivalence



The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

This can be computed as the projection of any vector which connects the origin to the plane onto the unit vector in the $\vec{G}_{hkl}$ direction. In this case, we choose, $\vec{a}_1/h$

General proof of Bragg-Laue equivalence



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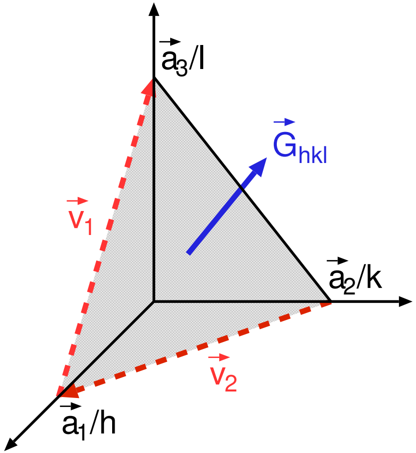

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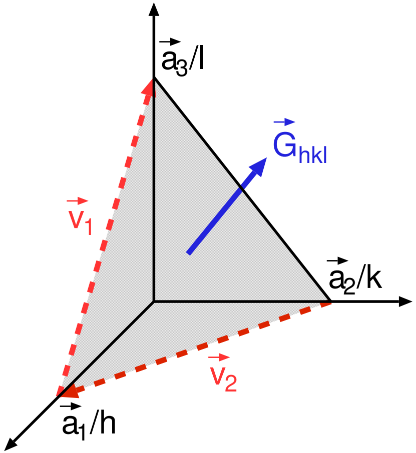

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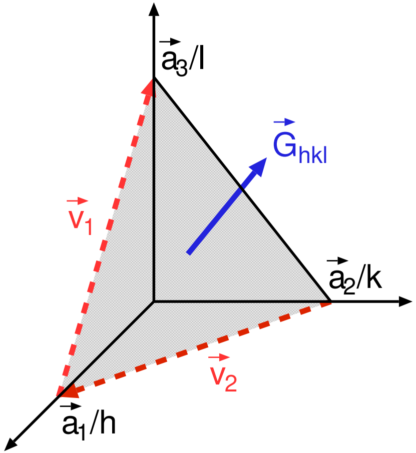

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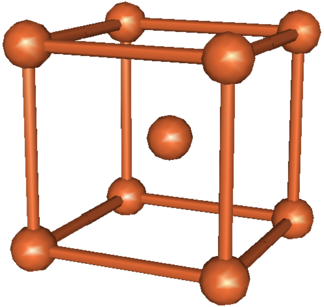
BCC structure factor

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



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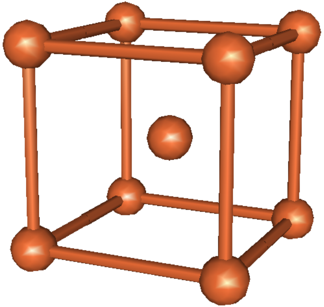

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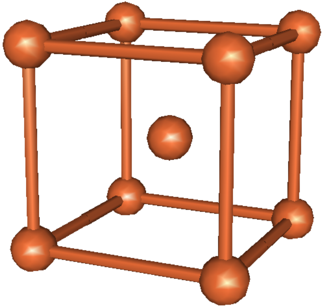
the unit cell structure factor is thus



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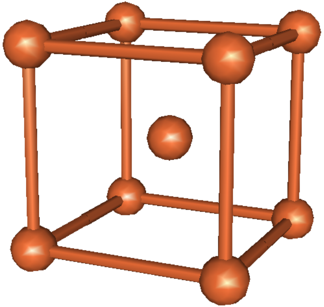
$$F^{bcc}_{hkl} = f(\vec{G}) \sum_j e^{i\vec{G}\cdot\vec{r}_j}$$



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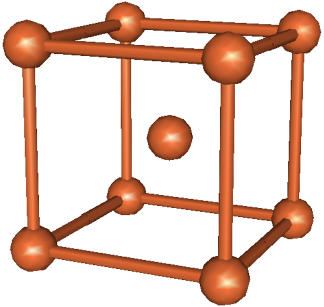
$$F_{hkl}^{bcc} = f(\vec{G}) \sum_j e^{i\vec{G}\cdot\vec{r}_j}$$

$$= f(\vec{G}) \left(1 + e^{i\pi(h+k+l)}\right)$$



BCC structure factor

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$$\vec{r}_1 = 0, \qquad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)$$

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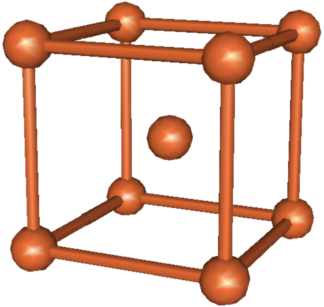

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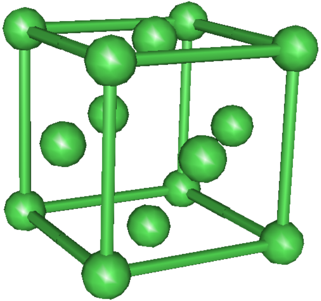

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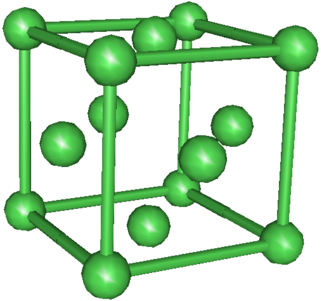

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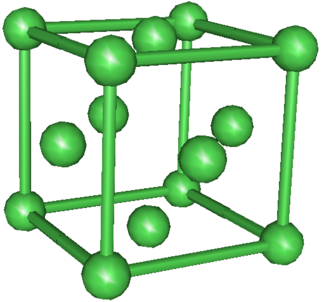

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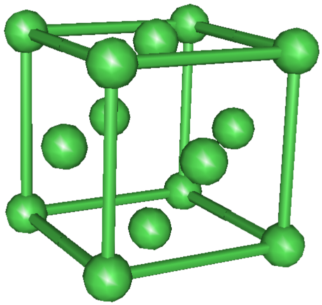

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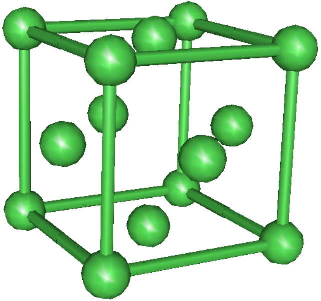

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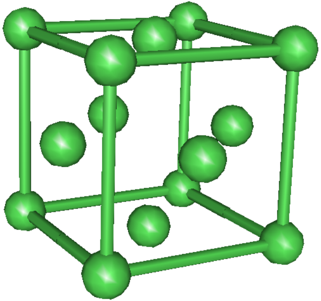
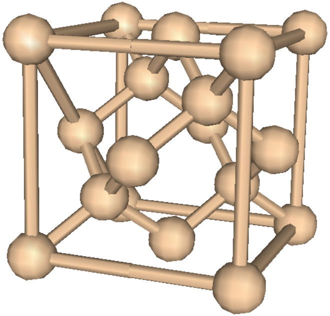


Diamond structure

This is a face centered cubic structure with two atoms in the basis which leads to 8 atoms in the conventional unit cell. These are located at



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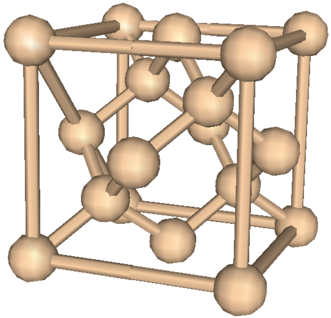

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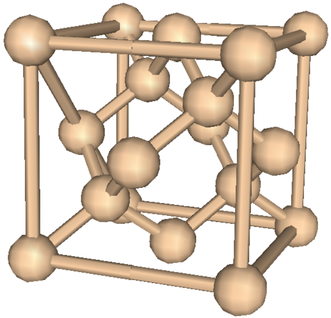
$$F_{hkl}^{diamond} = f(\vec{G})\Big(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k+l)/2} + e^{i\pi(3h+3k+l)/2} + e^{i\pi(h+3k+3l)/2} + e^{i\pi(3h+k+3l)/2}\Big)$$



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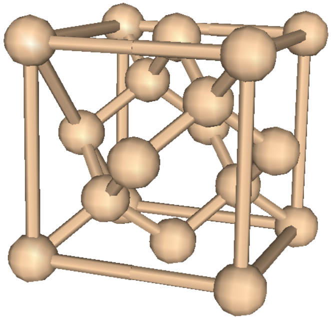
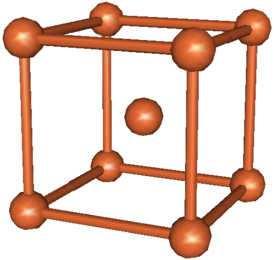


This is non-zero when h,k,l all even and $h+k+l = 4n$ or h,k,l all odd

Heteroatomic structures



← bcc

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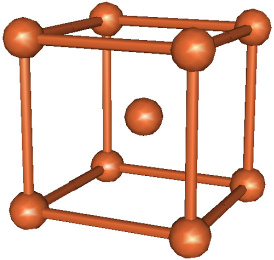

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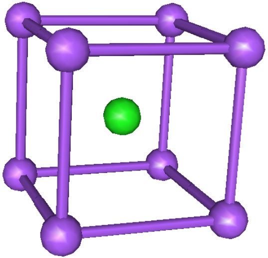
sc →



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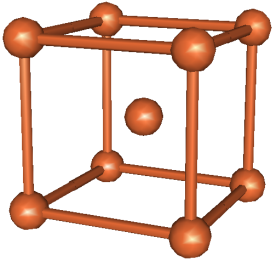

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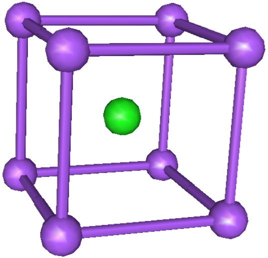

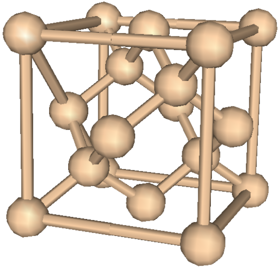

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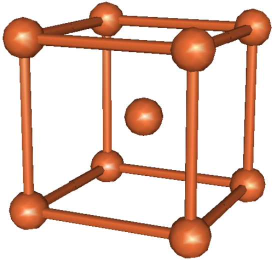

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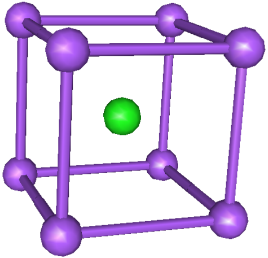

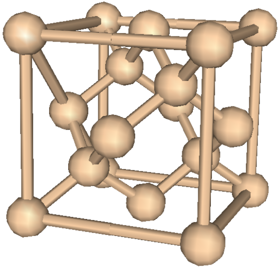

← diamond

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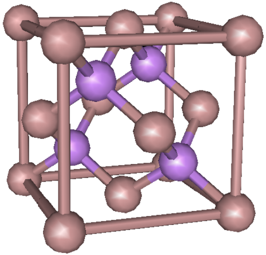

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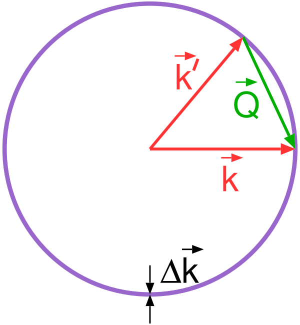

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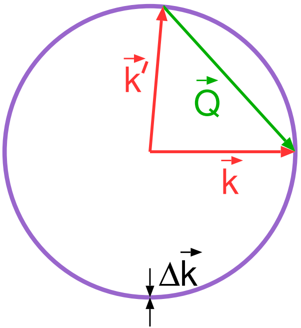

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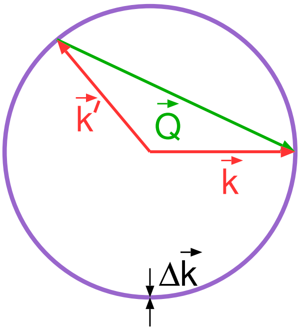

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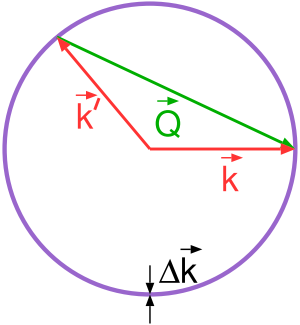

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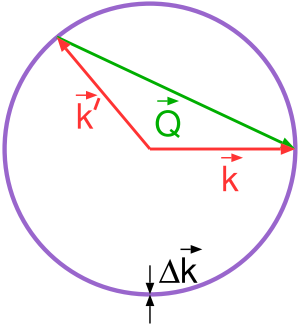

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http://www.phillipslab.org/software

Ewald sphere & the reciprocal lattice

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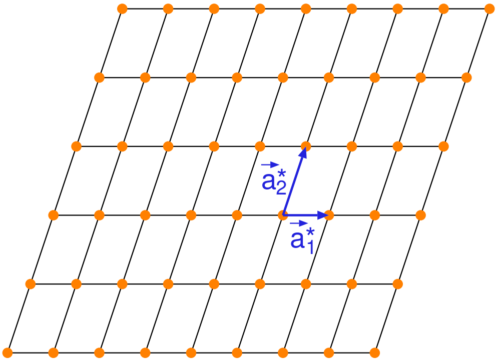

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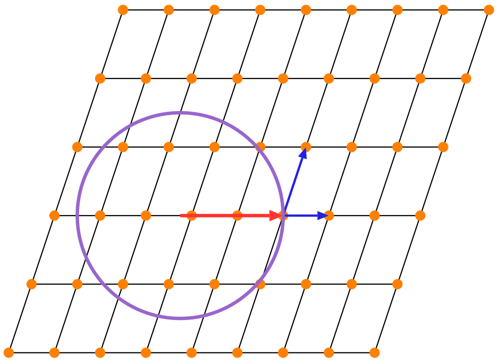

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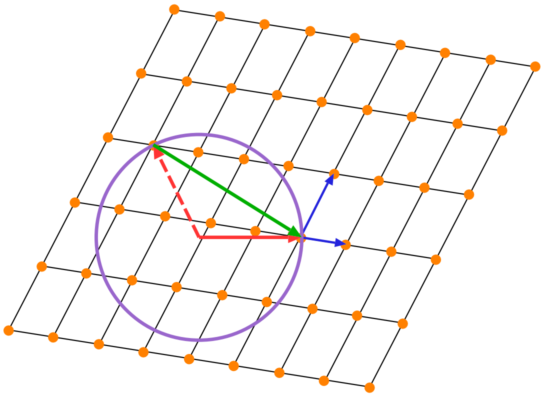

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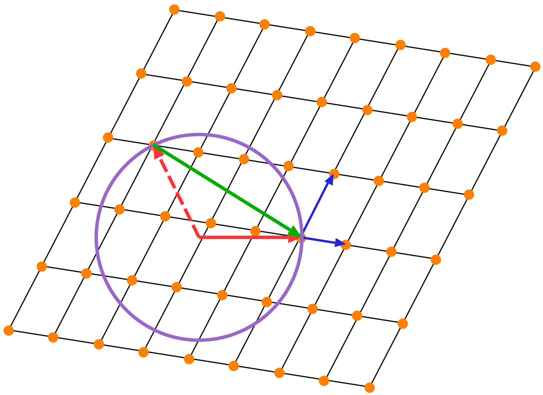

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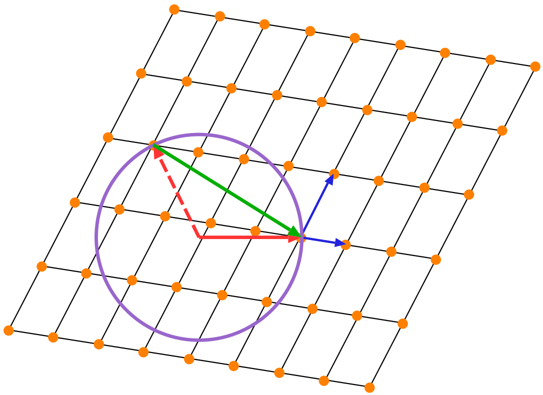

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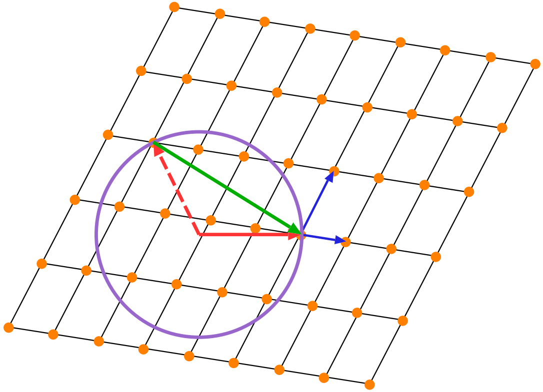
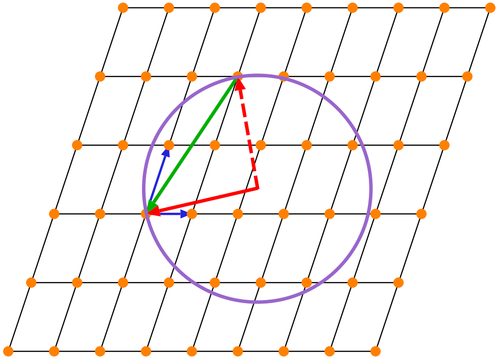


$$\vec{G}_{hlk} = h\vec{a}_1^* + k\vec{a}_2^*$$

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.



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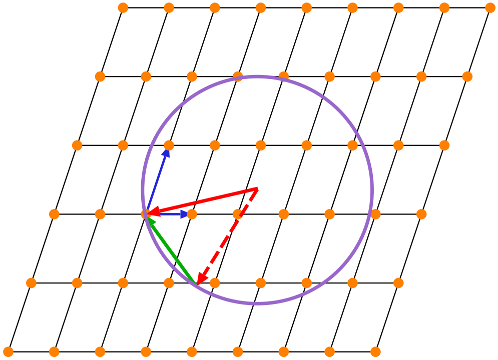
In directions of $\vec{k}'$ (detector position) where there is no reciprocal lattice point, there can be no diffraction peak.



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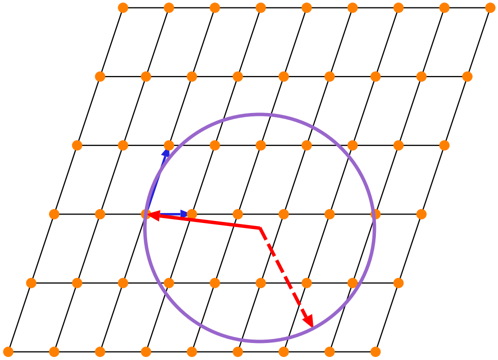
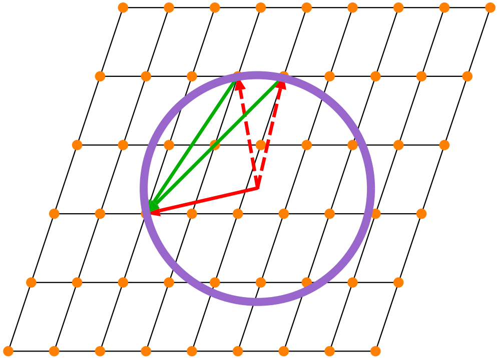
If the crystal is rotated slightly with respect to the incident beam, $\vec{k}$, there may be no Bragg reflections possible at all.



Polychromatic radiation

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



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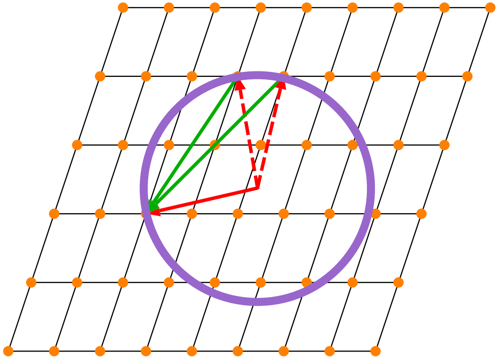

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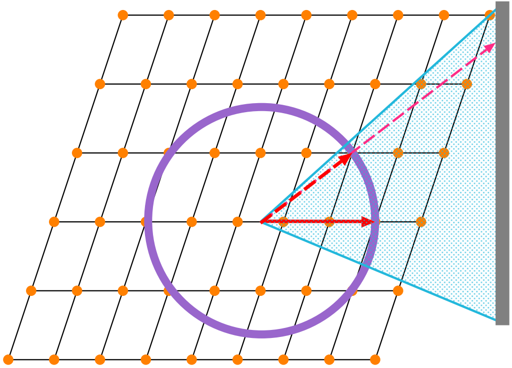
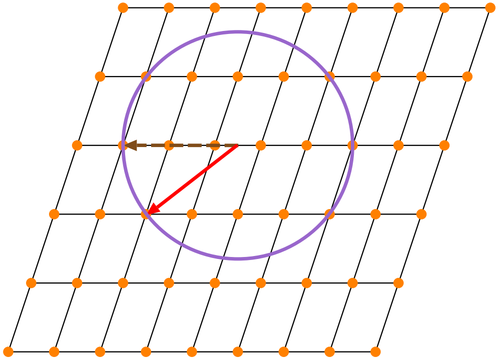
In protein crystallography, the area detector is in a fixed location with respect to the incident beam and the crystal is rotated on a spindle so that as Laue conditions are met, spots are produced on the detector at the diffraction angle



Multiple scattering

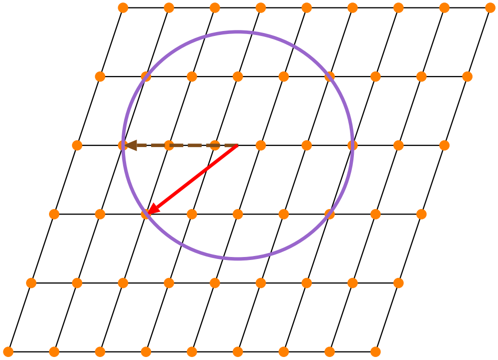
If more than one reciprocal lattice point is on the Ewald sphere, scattering can occur internal to the crystal.



Multiple scattering

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

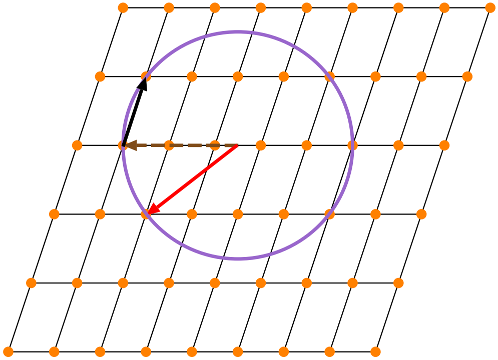
The xrays are first scattered along $\vec{k}_{int}$



Multiple scattering

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

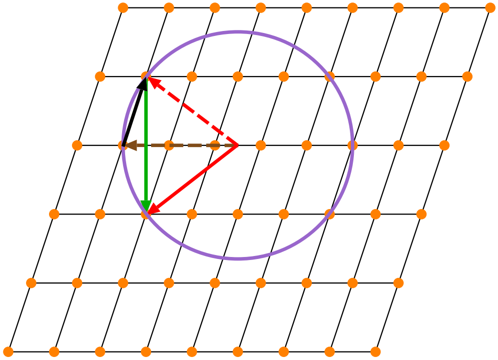
The xrays are first scattered along $\vec{k}_{int}$ then along the reciprocal lattice vector which connects the two points on the Ewald sphere, $\vec{G}$



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 $\vec{k}'$.



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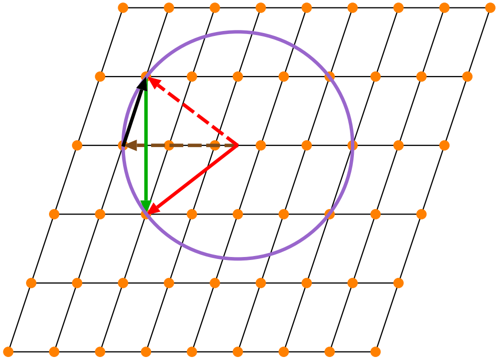
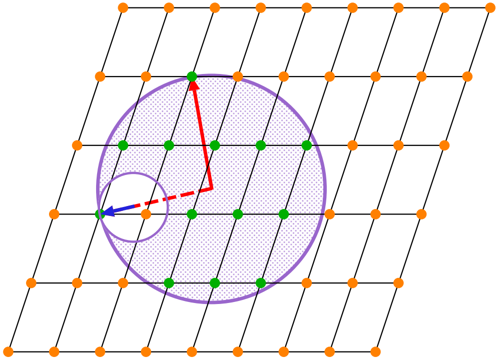
This is the cause of monochromator glitches which sometimes remove intensity but can also add intensity to the reflection the detector is set to measure.



Laue diffraction

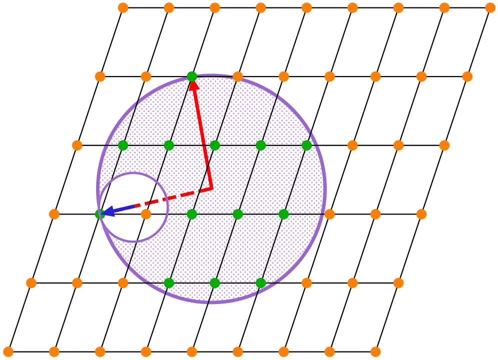
The Laue diffraction technique uses a wide range of radiation from $\vec{k}_{min}$ to $\vec{k}_{max}$



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.



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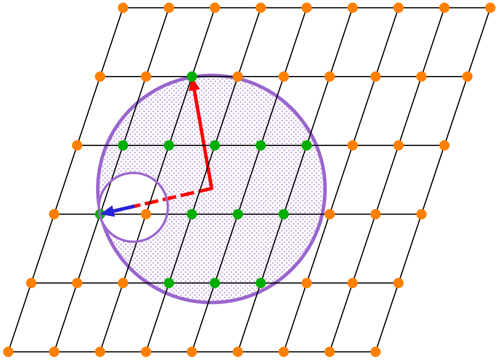
These define two Ewald spheres and a volume between them such that any reciprocal lattice point which lies in the volume will meet the Laue condition for reflection.

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

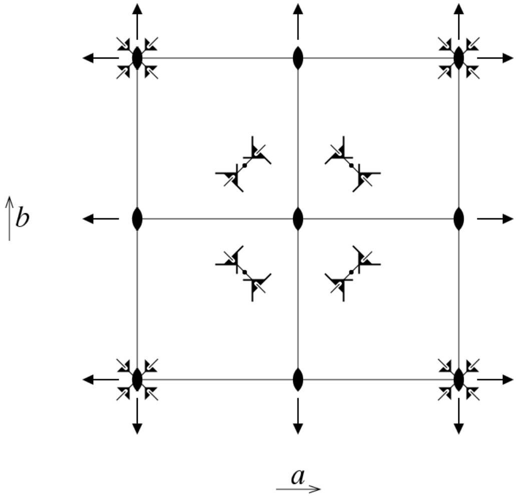
Exercise 1 - Ewald sphere

Exercise 4 - Wavelength

Exercise 8 - Laue diffraction

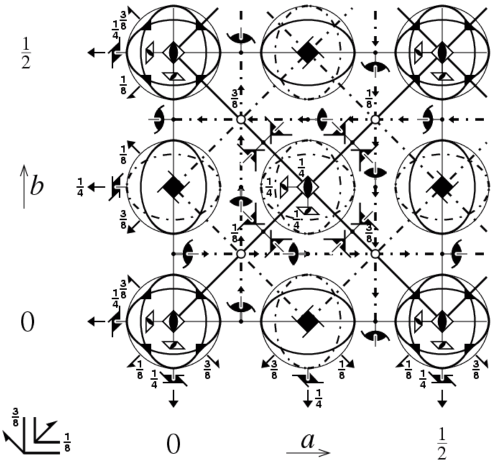
Exercise 9 - Serial crystallography

*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	$\frac14-x, \frac14-y, \frac14-z$
2	$x, \bar{y}, \bar{z}$	26	$\frac14-x, \frac14+y, \frac14+z$
3	$\bar{x}, y, \bar{z}$	27	$\frac14+x, \frac14-y, \frac14+z$
4	$\bar{x}, \bar{y}, z$	28	$\frac14+x, \frac14+y, \frac14-z$
5	z, x, y	29	$\frac14-z, \frac14-x, \frac14-y$
6	$\bar{z}, \bar{x}, y$	30	$\frac14+z, \frac14+x, \frac14-y$
7	$z, \bar{x}, \bar{y}$	31	$\frac14-z, \frac14+x, \frac14+y$
8	$\bar{z}, x, \bar{y}$	32	$\frac14+z, \frac14-x, \frac14+y$
9	y, z, x	33	$\frac14-y, \frac14-z, \frac14-x$
10	$\bar{y}, z, \bar{x}$	34	$\frac14+y, \frac14-z, \frac14+x$
11	$\bar{y}, \bar{z}, x$	35	$\frac14+y, \frac14+z, \frac14-x$
12	$y, \bar{z}, \bar{x}$	36	$\frac14-y, \frac14+z, \frac14+x$
13	$\frac14+x, \frac14-z, \frac14+y$	37	$\bar{x}, z, \bar{y}$
14	$\frac14+x, \frac14+z, \frac14-y$	38	$\bar{x}, \bar{z}, y$
15	$\frac14-x, \frac14-z, \frac14-y$	39	x, z, y
16	$\frac14-x, \frac14+z, \frac14+y$	40	$x, \bar{z}, \bar{y}$
17	$\frac14+z, \frac14+y, \frac14-x$	41	$\bar{z}, \bar{y}, x$
18	$\frac14-z, \frac14+y, \frac14+x$	42	$z, \bar{y}, \bar{x}$
19	$\frac14-z, \frac14-y, \frac14-x$	43	z, y, x
20	$\frac14+z, \frac14-y, \frac14+x$	44	$\bar{z}, y, \bar{x}$
21	$\frac14-y, \frac14+x, \frac14+z$	45	$y, \bar{x}, \bar{z}$
22	$\frac14+y, \frac14-x, \frac14+z$	46	$\bar{y}, x, \bar{z}$
23	$\frac14-y, \frac14-x, \frac14-z$	47	y, x, z
24	$\frac14+y, \frac14+x, \frac14-z$	48	$\bar{y}, \bar{x}, z$

$+ (0,\frac12,\frac12), (\frac12,0,\frac12), (\frac12,\frac12,0)$

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-3m*) [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)