Today's outline - October 09, 2024

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Reading Assignment: Chapter 5.4

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Homework Assignment #04:
Chapter 4: 2,4,6,7,10
due Monday, October 14, 2024

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Reading Assignment: Chapter 5.4

Homework Assignment #04:
Chapter 4: 2,4,6,7,10
due Monday, October 14, 2024

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Monday, October 28, 2024

Scattering from ordered crystals

Liquid scattering and small angle scattering provide structural information about highly disordered systems and long length scales, respectively.

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We will now proceed to develop a model for this kind of scattering starting with some definitions in 2D space.

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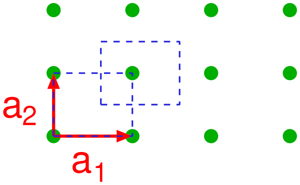

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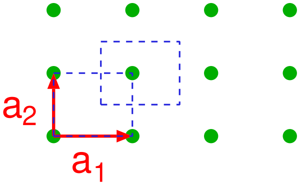

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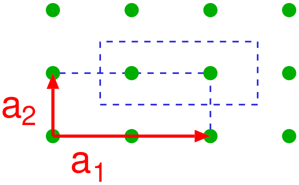

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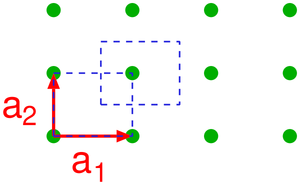

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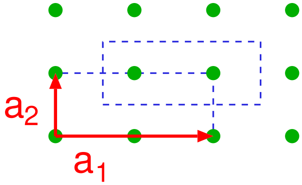

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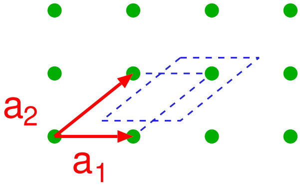

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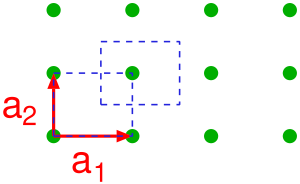

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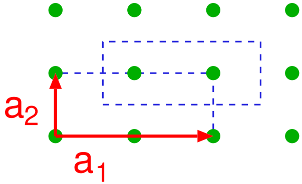

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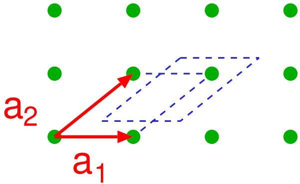

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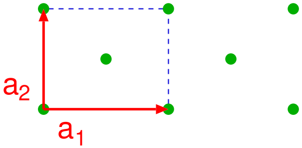

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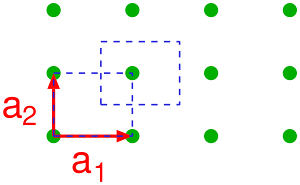

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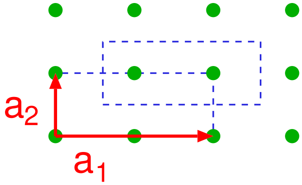

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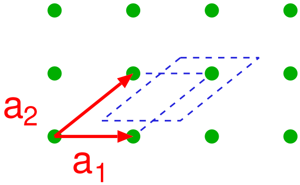

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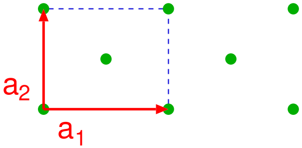

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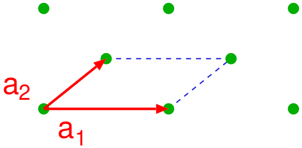

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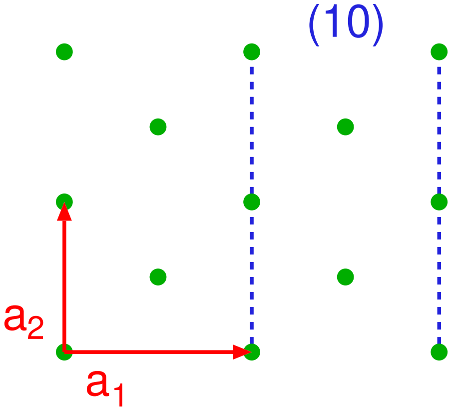
Miller indices



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$$\frac{a_1}{h}, \quad \frac{a_2}{k}$$

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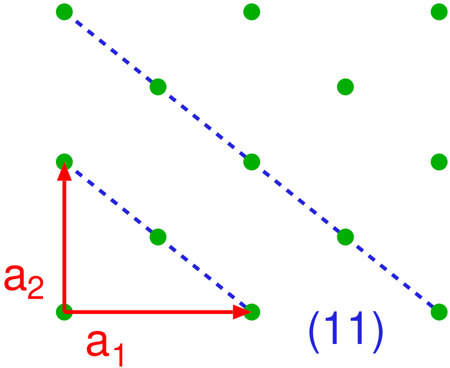

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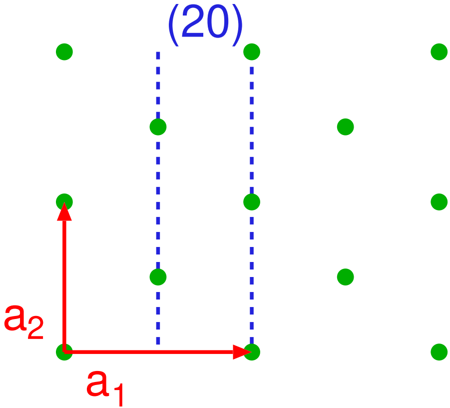

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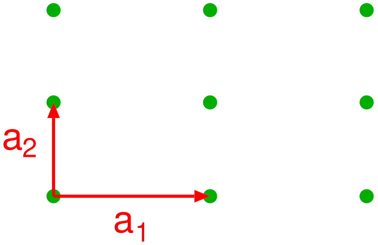
for a lattice with orthogonal unit vectors

$$\frac{1}{d_{hk}^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2}$$

Reciprocal lattice



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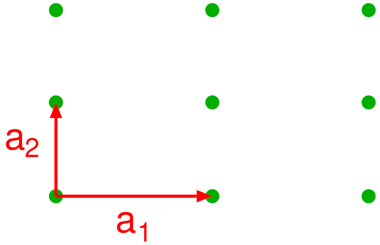

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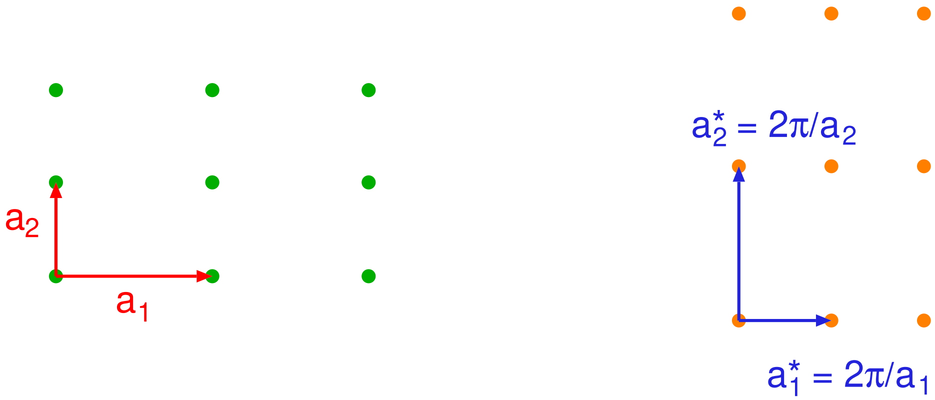

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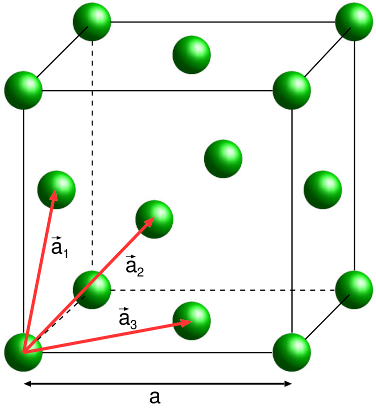
$$\therefore\ \vec{Q} = \vec{G}_{hkl}$$

The FCC reciprocal lattice

The primitive lattice vectors of the face-centered cubic lattice are



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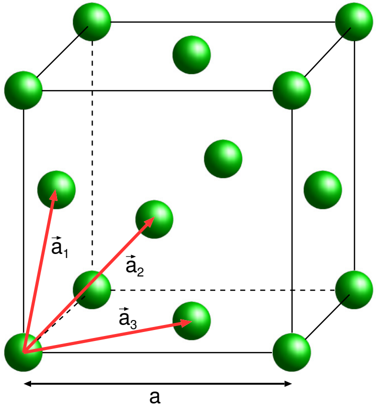

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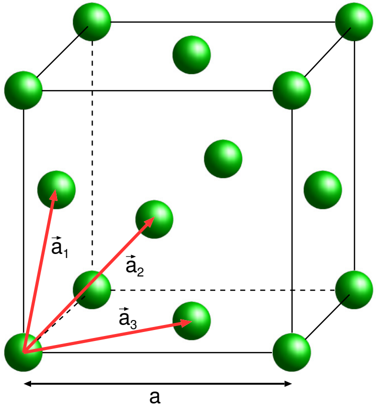

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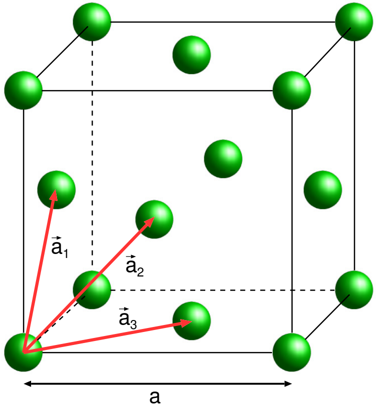

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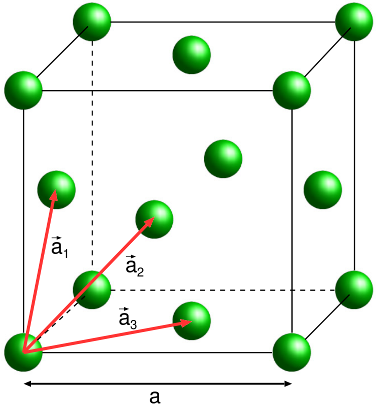

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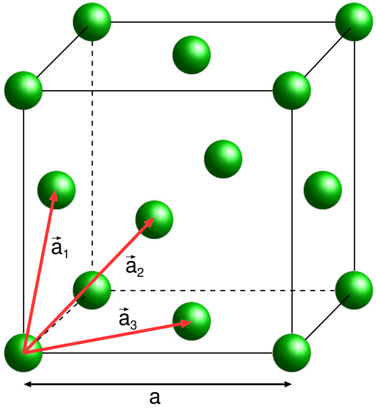

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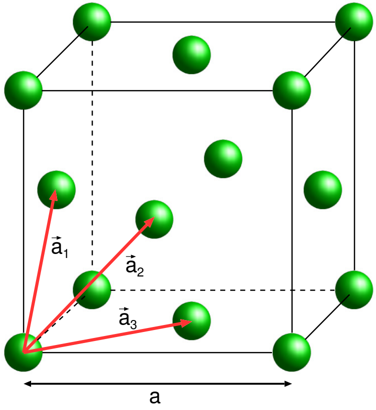

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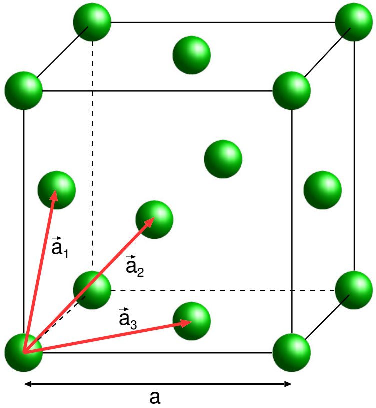

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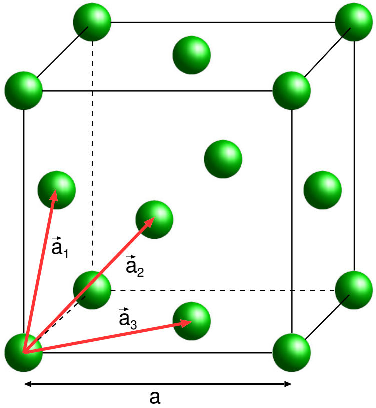

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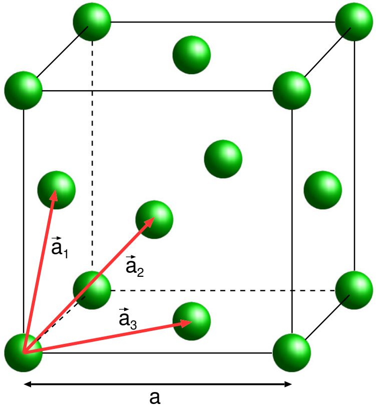

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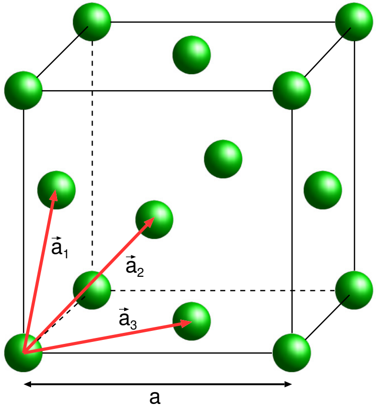

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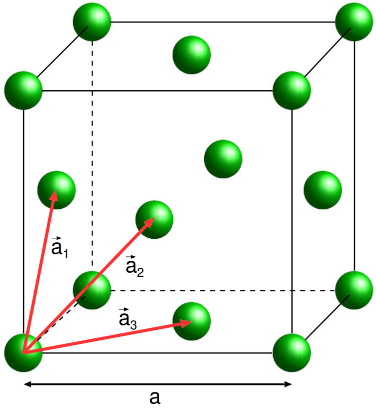

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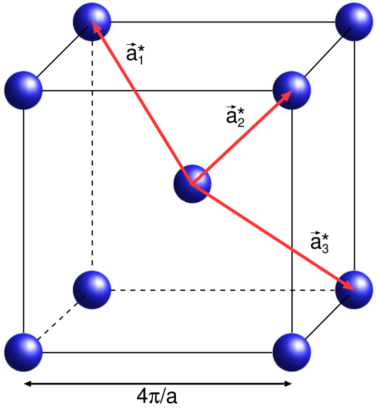

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the numerator can be simplified as

$$\sin(N\pi[h+\xi]) = \cancelto{0}{\sin(N\pi h)}\cos(N\pi\xi) + \cancelto{1}{\cos(N\pi h)}\sin(N\pi\xi) = \pm\sin(N\pi\xi)$$

the peak height can be estimated for small ξ as

$$|S_N(Q)| = \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} \approx \frac{N\pi\xi}{\pi\xi} \to N \quad \text{as} \quad \xi \to 0$$

and the half width measured at the first minimum of the lattice sum

$$|S_N(Q)| \to 0, \qquad N\pi\xi = \pi, \qquad \xi_{1/2} \approx \frac{1}{2N}$$

Lattice sum in 1D

the peak area can be obtained by integration

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since $\delta(a^*\xi) = \delta(\xi)/a^*$

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the 1D modulus squared

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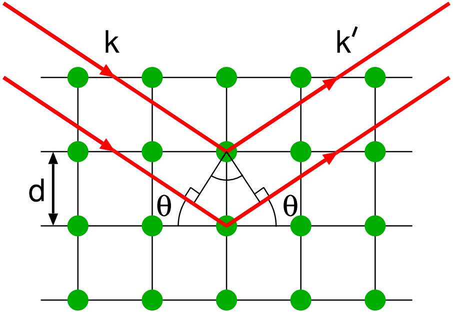
$$\left|S_N(\vec{Q})\right|^2 \rightarrow NV_c^* \sum_{\vec{G}_{hkl}} \delta(\vec{Q} - \vec{G}_{hkl})$$

Bragg condition



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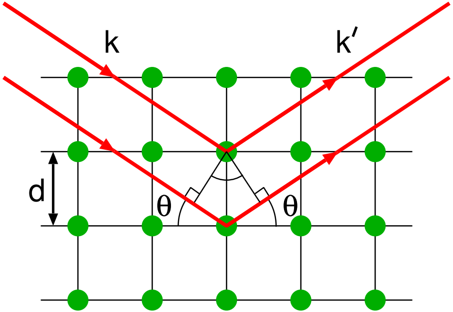
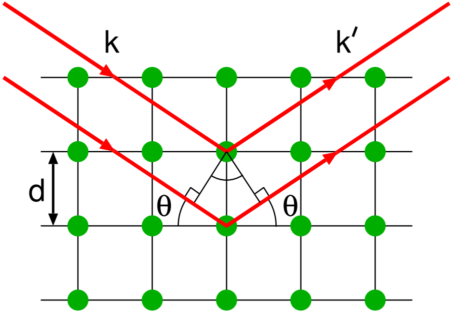


The Bragg condition for diffraction is derived by assuming specular reflection from parallel planes separated by a distance d.

Bragg condition



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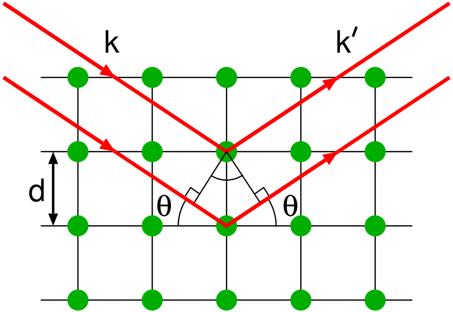

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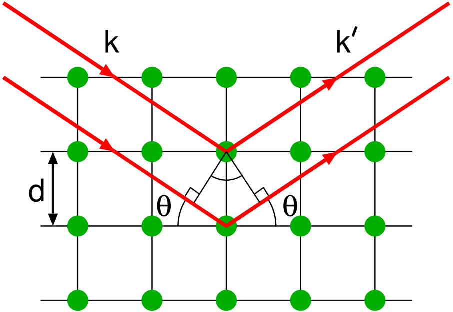

$$2d \sin\theta = \lambda$$

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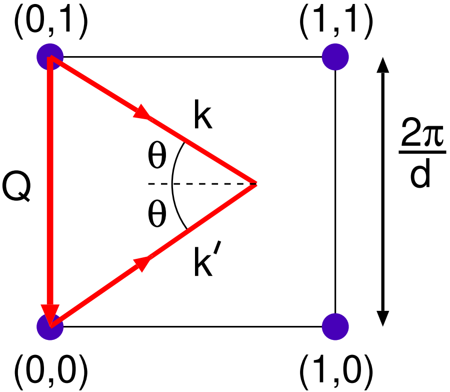
Laue condition

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



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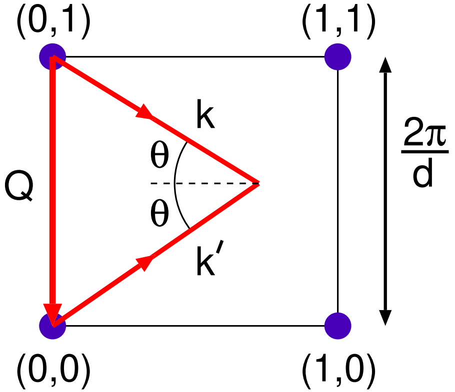

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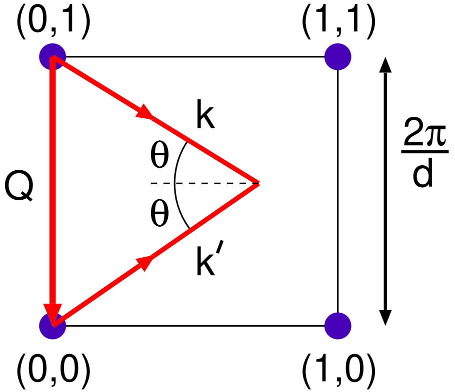

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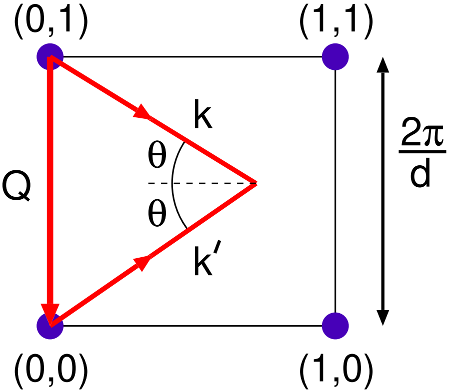

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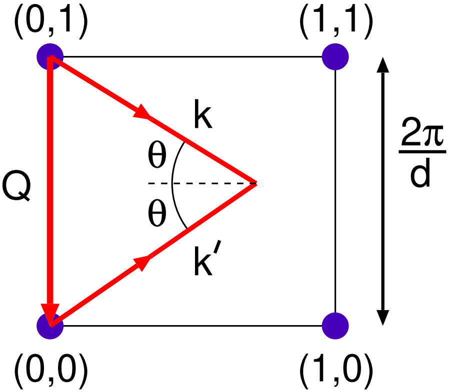

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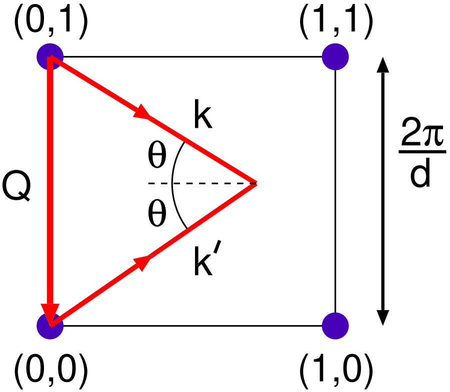

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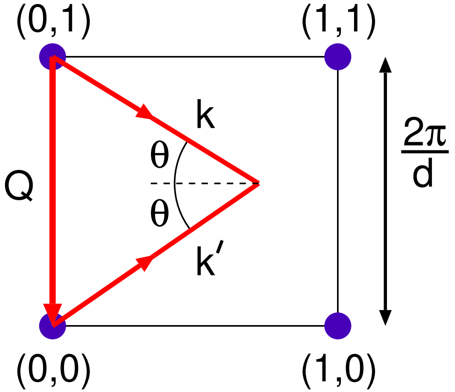

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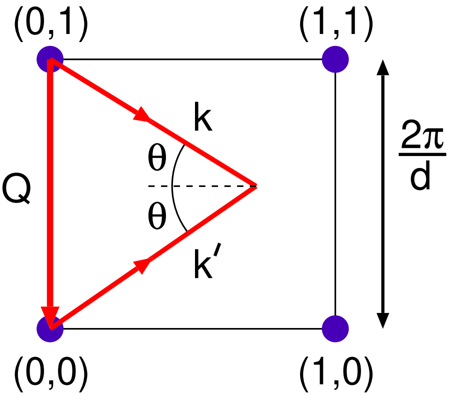
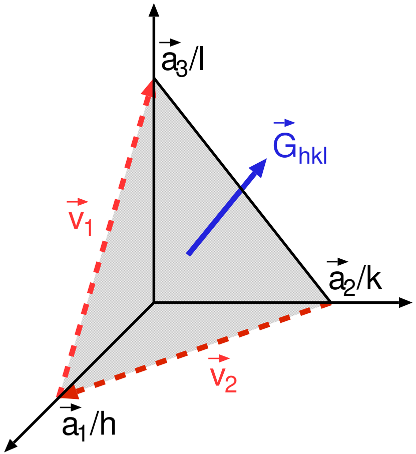
Thus the Bragg and Laue conditions are equivalent



General proof of Bragg-Laue equivalence



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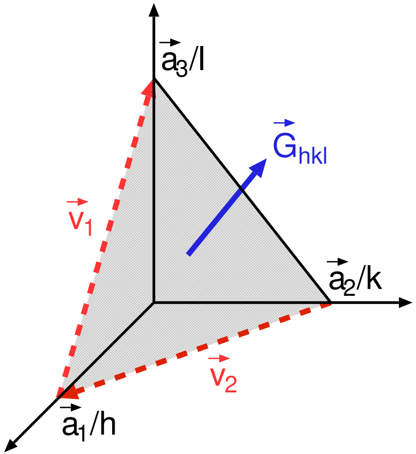

Must show that for each point in reciprocal space, there exists a set of planes in the real space lattice such that:

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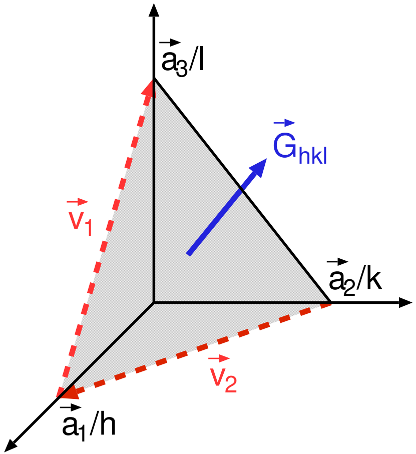

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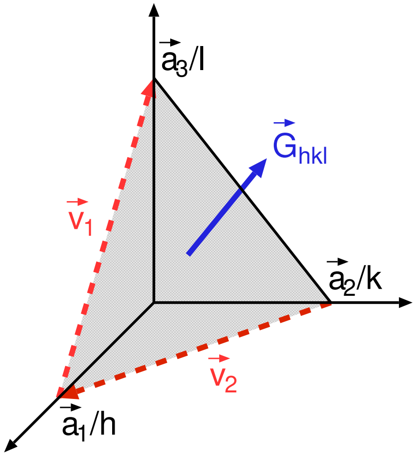

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$$|\vec{G}_{hkl}| = \frac{2\pi}{d_{hkl}}$$

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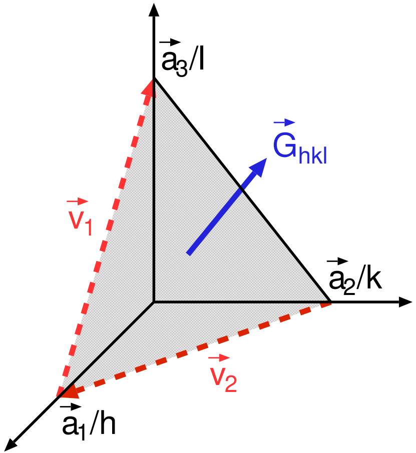

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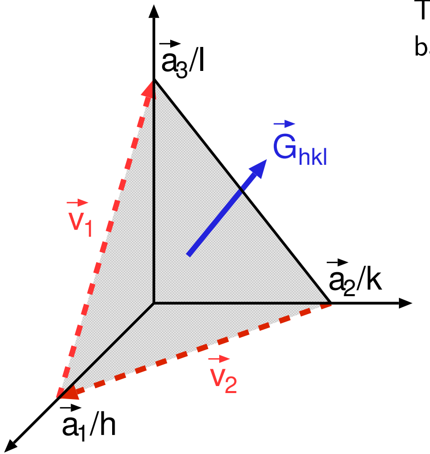

The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

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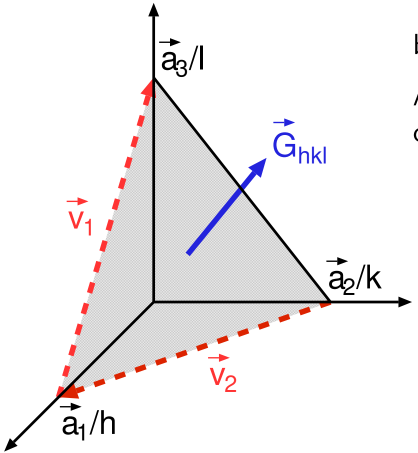

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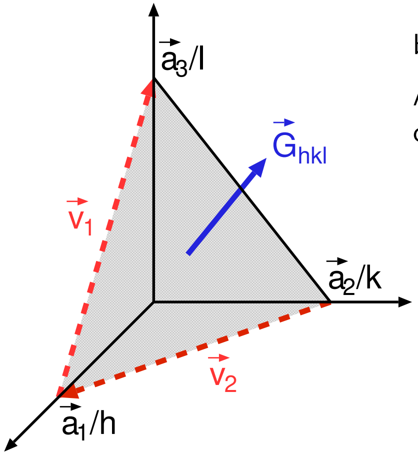

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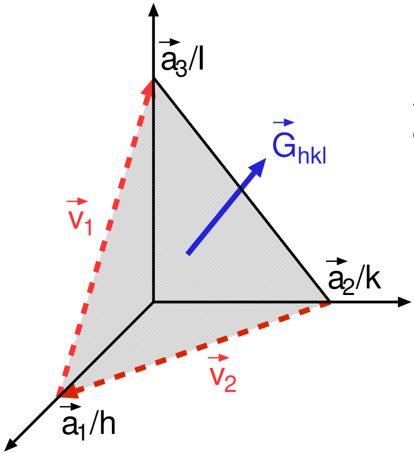

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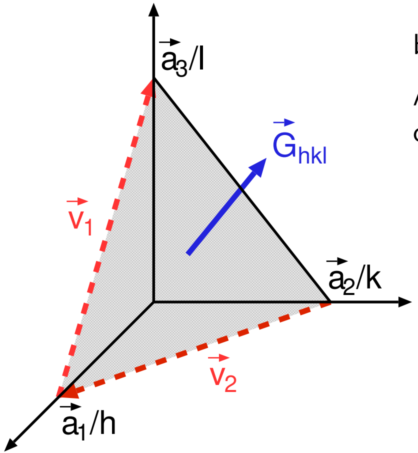

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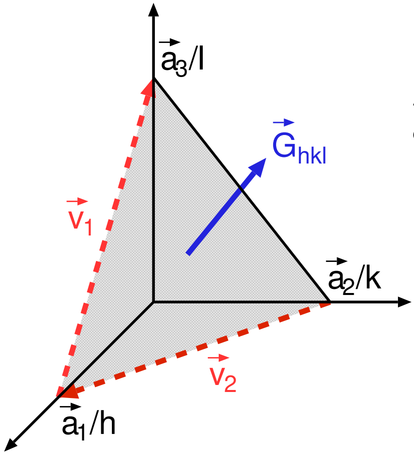

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$$\vec{G}_{hkl} \cdot \vec{v} = (h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*) \cdot \left((\epsilon_2 - \epsilon_1)\frac{\vec{a}_1}{h} - \epsilon_2 \frac{\vec{a}_2}{k} + \epsilon_1 \frac{\vec{a}_3}{l} \right)$$

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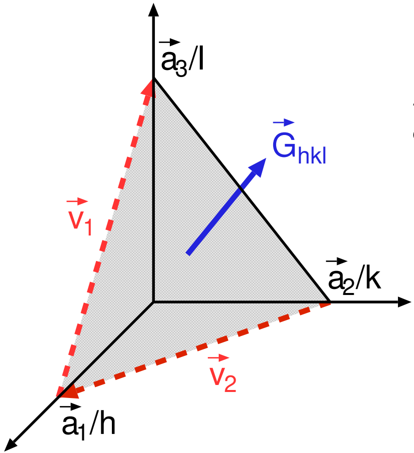

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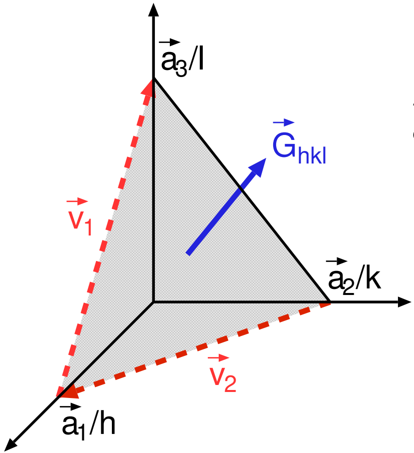
$$= 2\pi(\epsilon_2 - \epsilon_1 - \epsilon_2 + \epsilon_1) = 0$$

General proof of Bragg-Laue equivalence



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

Any vector, $\vec{v}$, in this plane can be expressed as a linear combination of two non-parallel vectors, $\vec{v}_1$ and $\vec{v}_2$

$$\vec{v}_1 = \frac{\vec{a}_3}{l} - \frac{\vec{a}_1}{h}, \quad \vec{v}_2 = \frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}$$

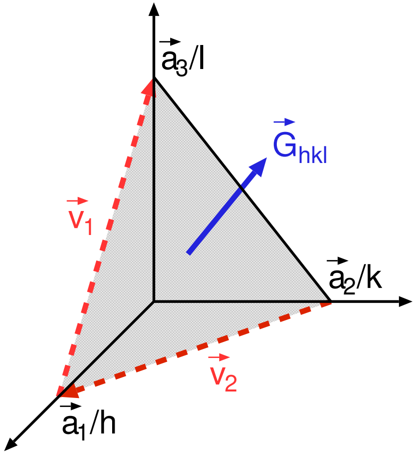
$$\vec{v} = \epsilon_1 \vec{v}_1 + \epsilon_2 \vec{v}_2$$

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

$$= 2\pi(\epsilon_2 - \epsilon_1 - \epsilon_2 + \epsilon_1) = 0$$

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

General proof of Bragg-Laue equivalence



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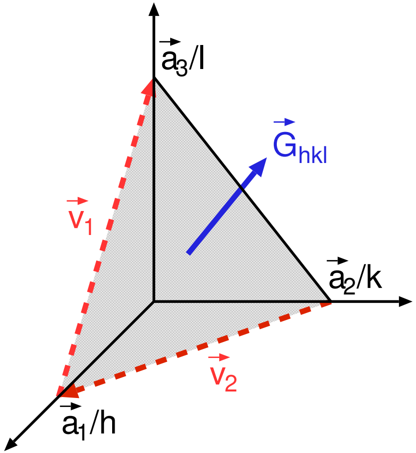
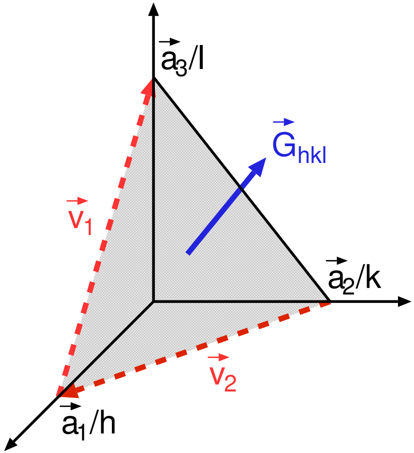


The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

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, $\vec{a}_1/h$

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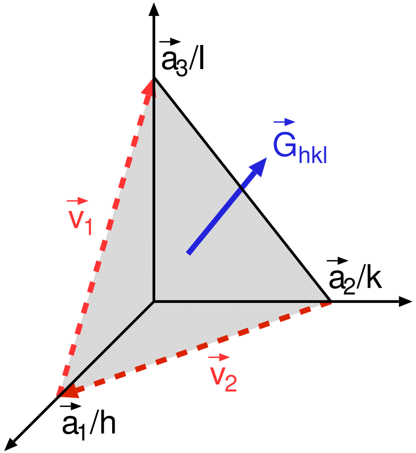

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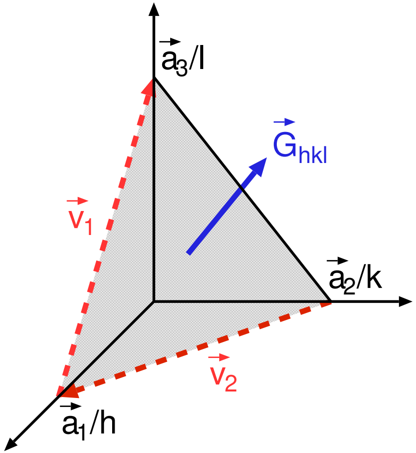

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$$\hat{G}_{hkl} \cdot \frac{\vec{a}_1}{h} = \frac{(h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*)}{|\vec{G}_{hkl}|} \cdot \frac{\vec{a}_1}{h}$$

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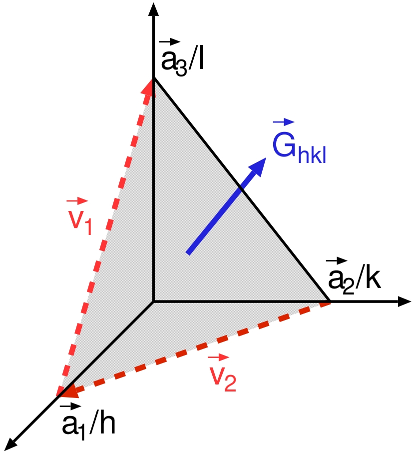

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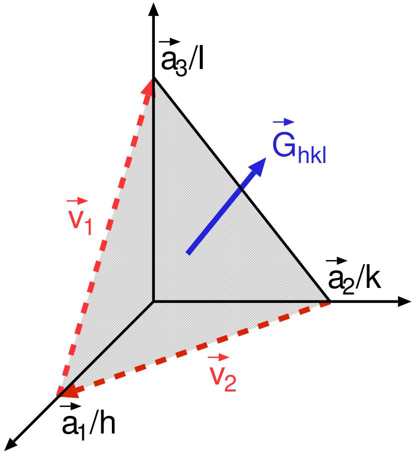

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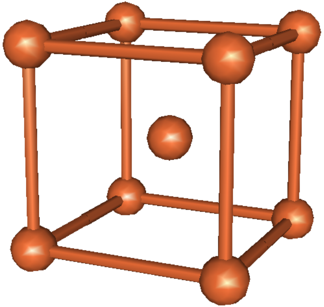
BCC structure factor

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



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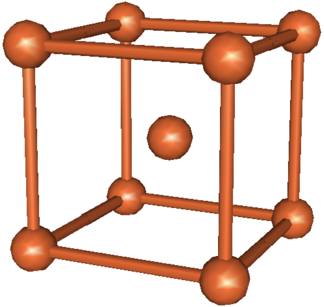

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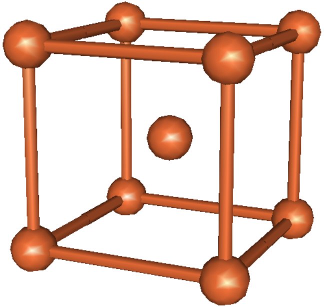

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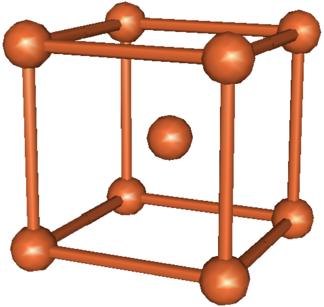

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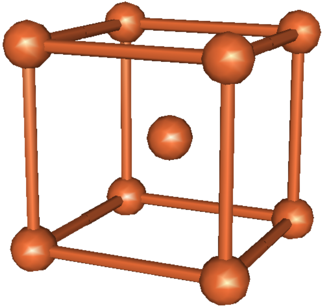

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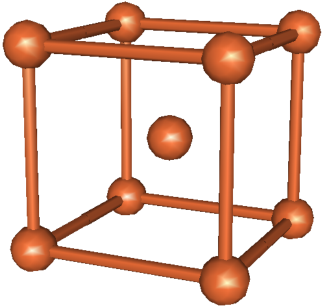

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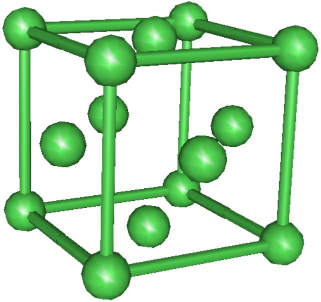
In the face-centered cubic structure, there are 4 atoms in the conventional, cubic unit cell. These are located at



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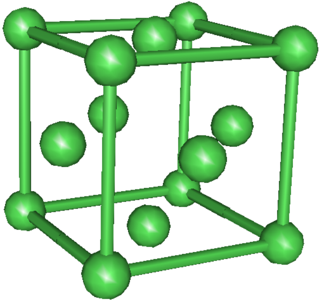

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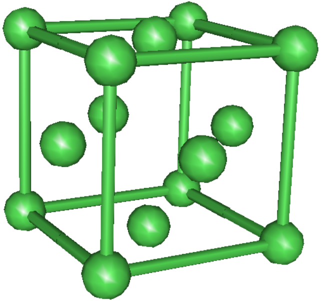

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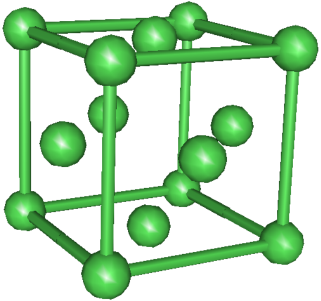

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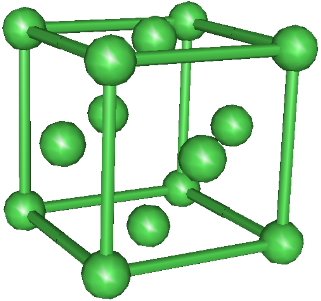

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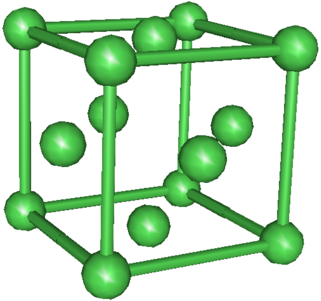
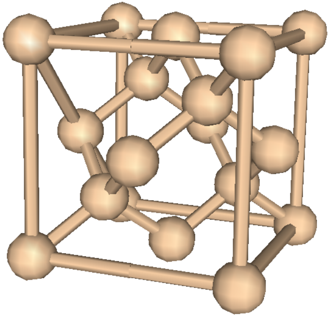


Diamond structure

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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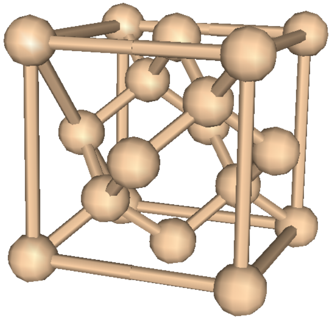
$$\vec{r}_6 = \frac{1}{4}(3\vec{a}_1 + 3\vec{a}_2 + \vec{a}_3), \quad \vec{r}_7 = \frac{1}{4}(\vec{a}_1 + 3\vec{a}_2 + 3\vec{a}_3), \quad \vec{r}_8 = \frac{1}{4}(3\vec{a}_1 + \vec{a}_2 + 3\vec{a}_3)$$



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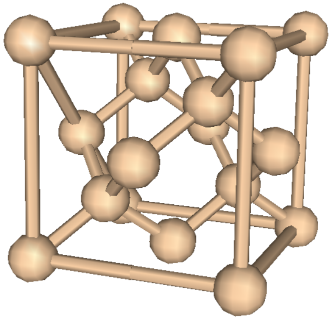
$$F_{hkl}^{diamond} = f(\vec{G})\Big(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k+l)/2} + e^{i\pi(3h+3k+l)/2} + e^{i\pi(h+3k+3l)/2} + e^{i\pi(3h+k+3l)/2}\Big)$$



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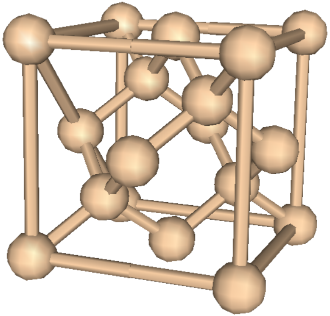
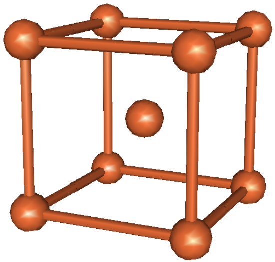
This is non-zero when h,k,l all even and $h+k+l = 4n$ or h,k,l all odd



Heteroatomic structures



← bcc

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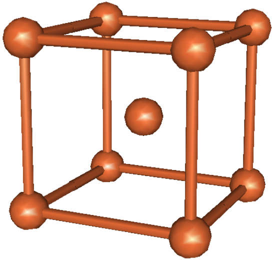
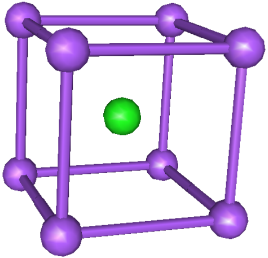


← bcc

sc →



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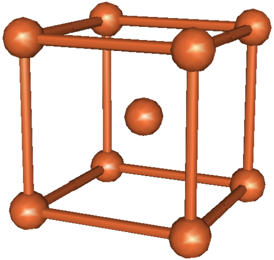

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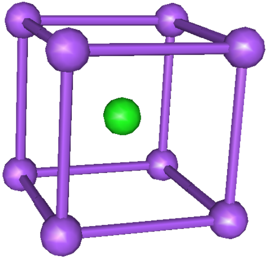

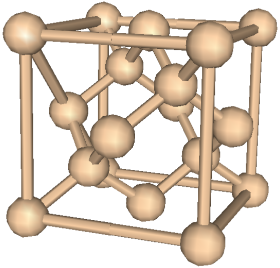

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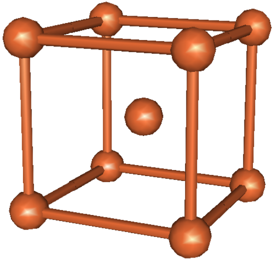

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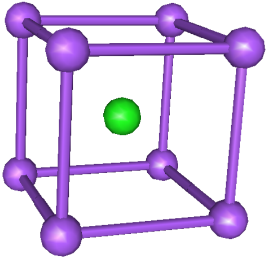

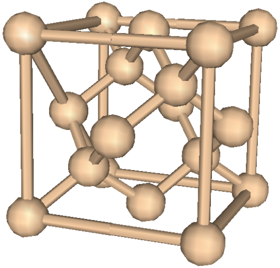

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fcc →