Today's Outline - March 05, 2015

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- Lattice & Basis Functions

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- Reciprocal Lattice for FCC

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- Crystal structure factor

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Reading assignment: Chapter 5.2

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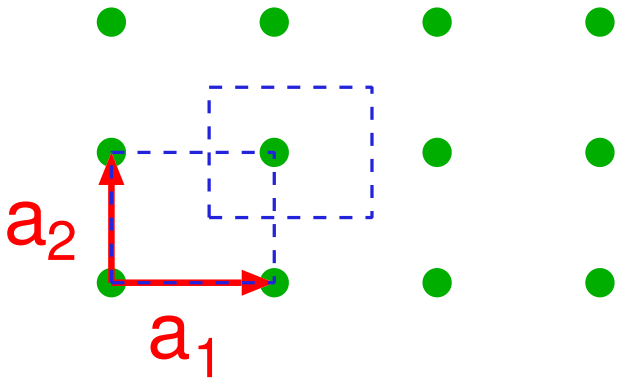
Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Tuesday, March 10, 2015

Types of lattice vectors

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2$$

Types of lattice vectors



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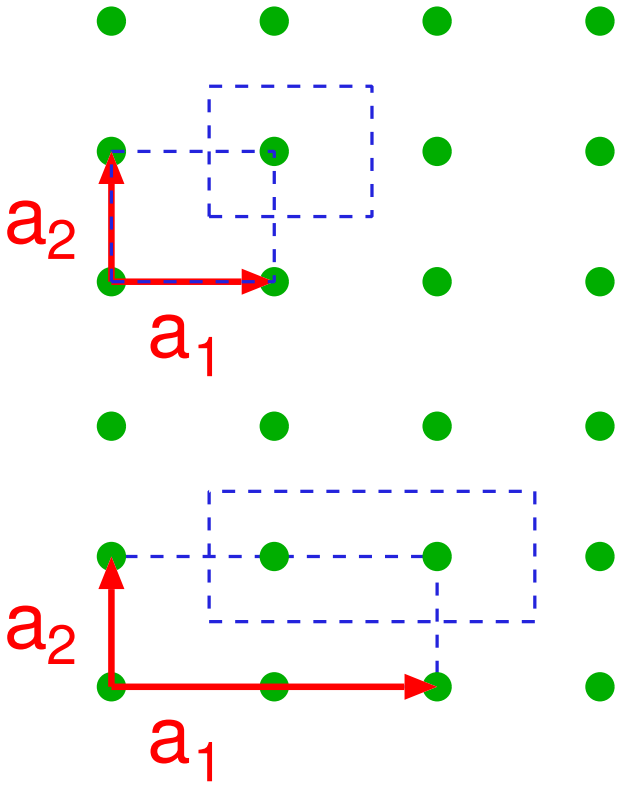
primitive

Types of lattice vectors



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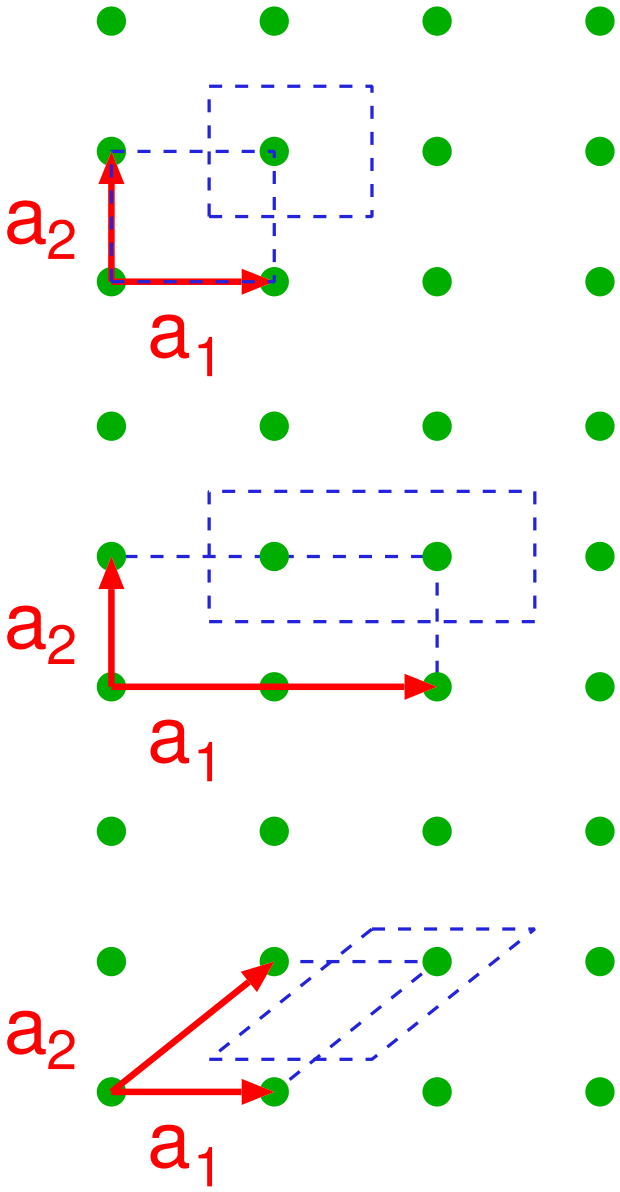


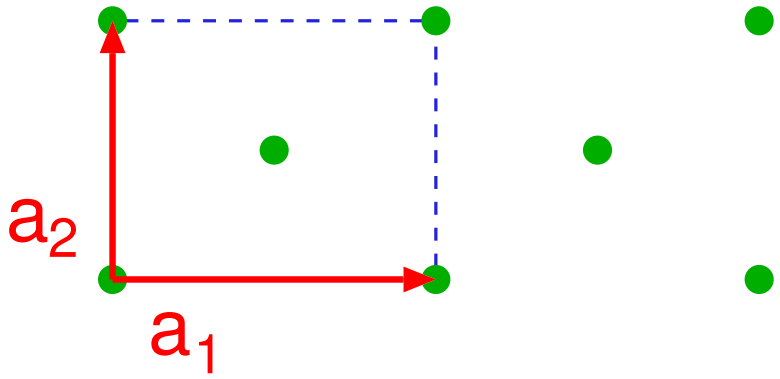
$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2$$

primitive

non-primitive

non-conventional

More about lattice vectors



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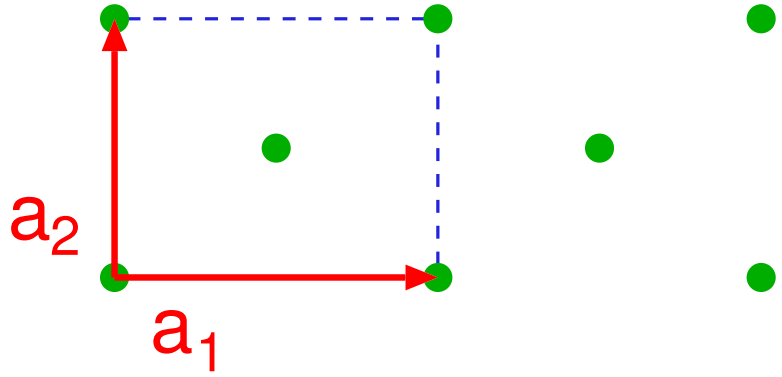
More about lattice vectors



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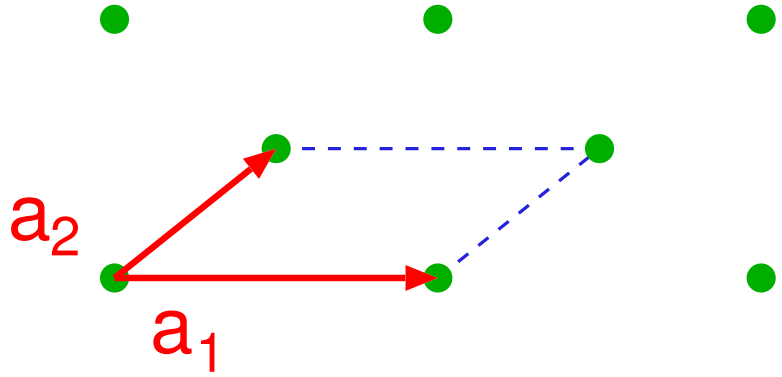
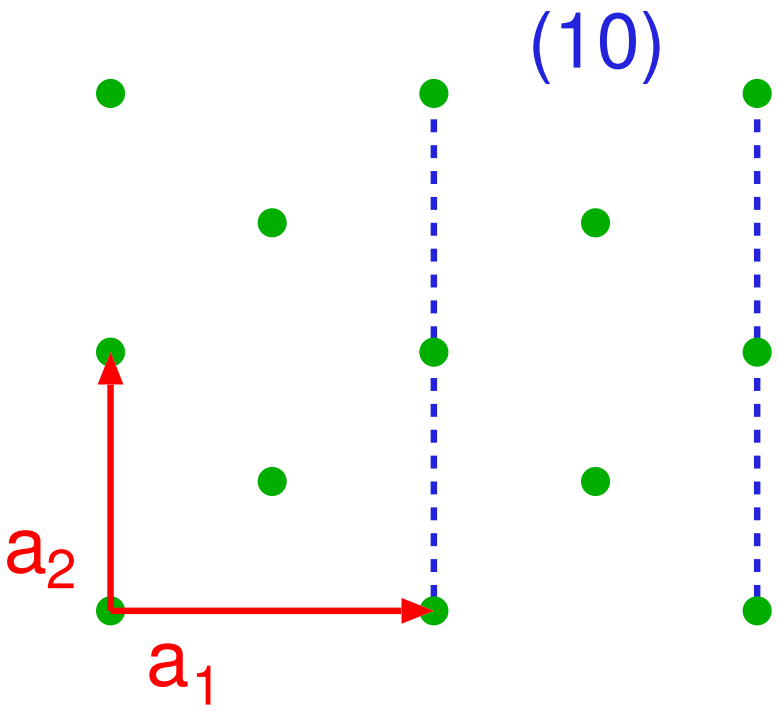


...are not primitive

Miller indices



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

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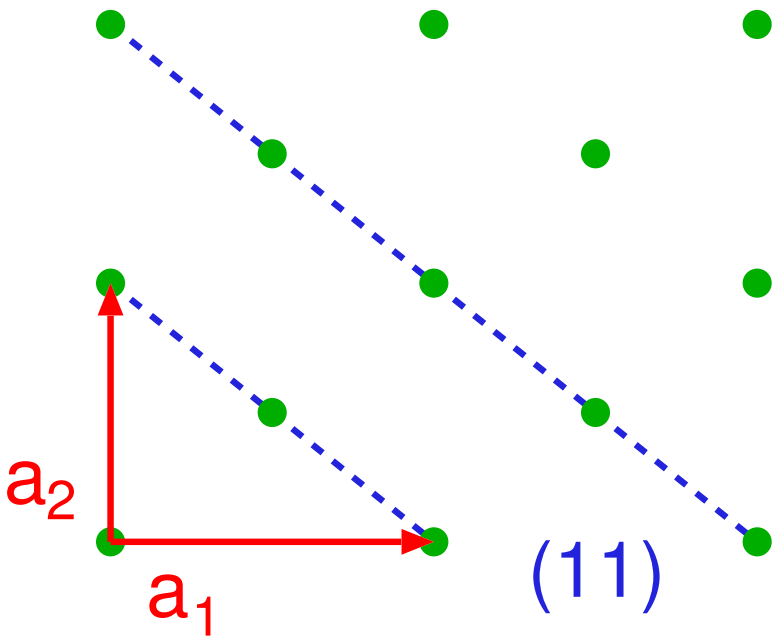

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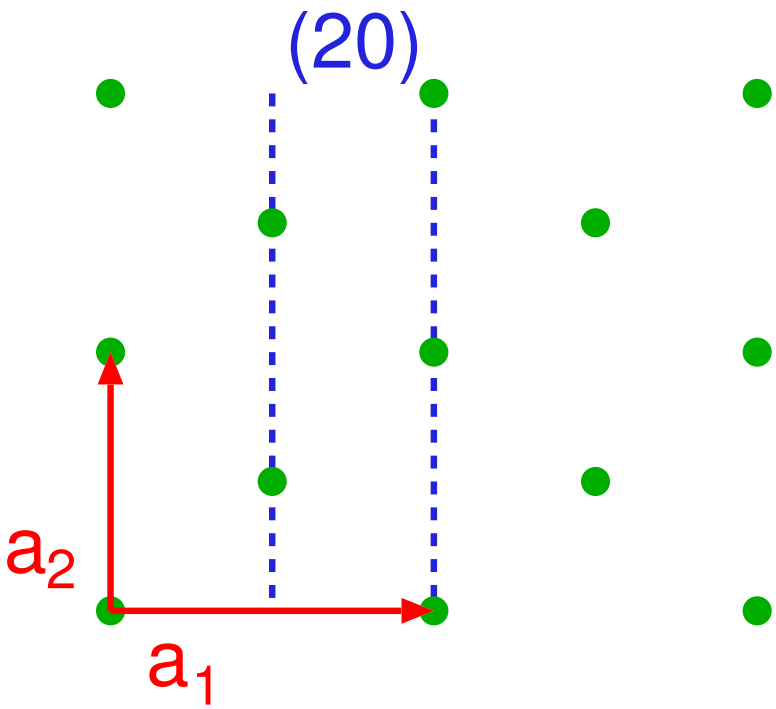

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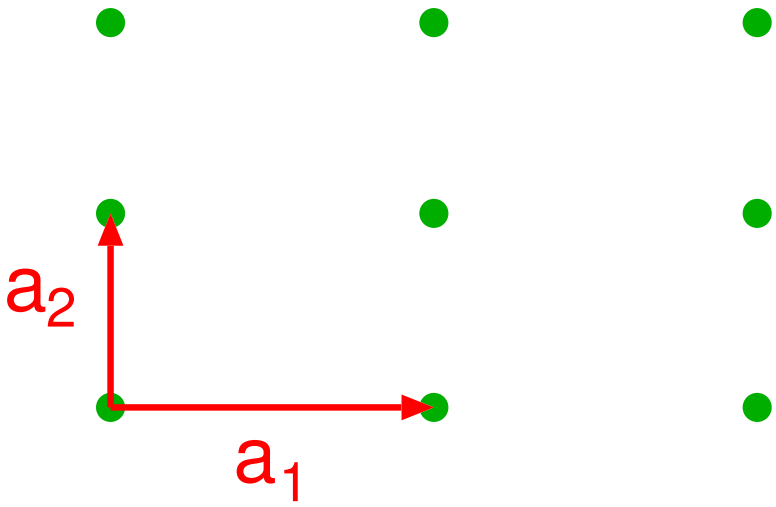
for a lattice with orthogonal unit vectors

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

Reciprocal lattice



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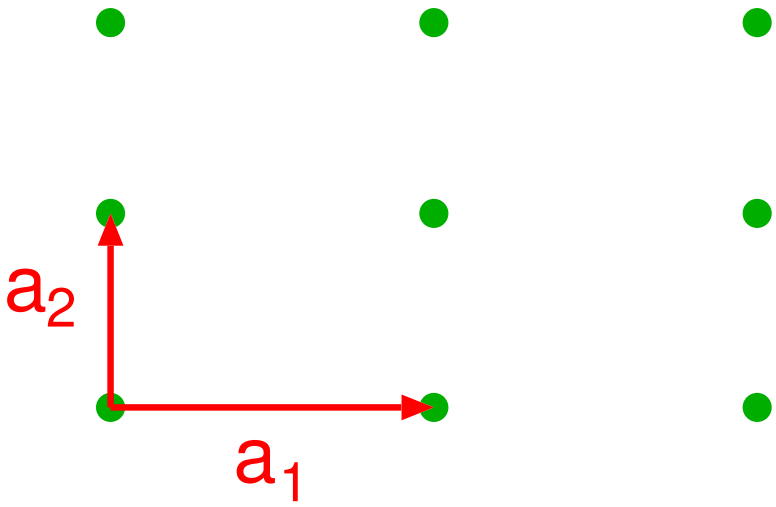

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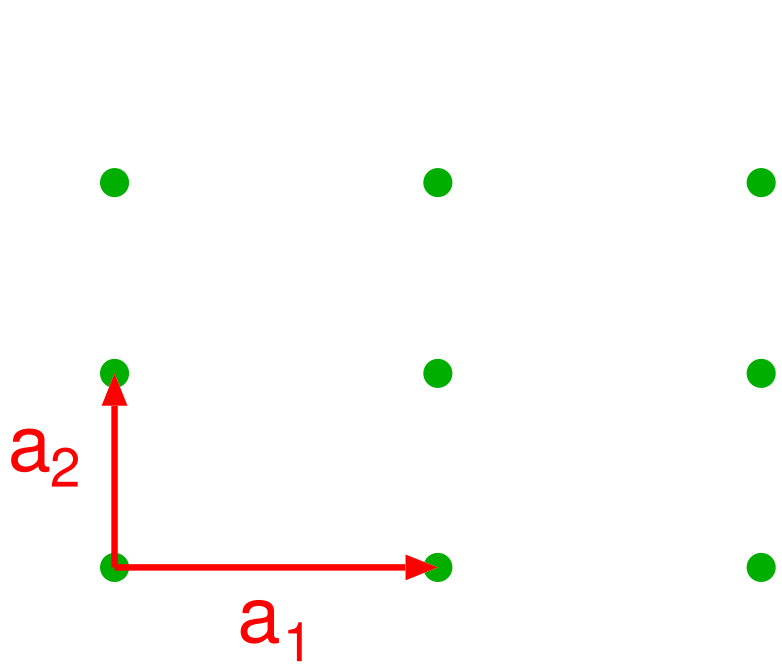

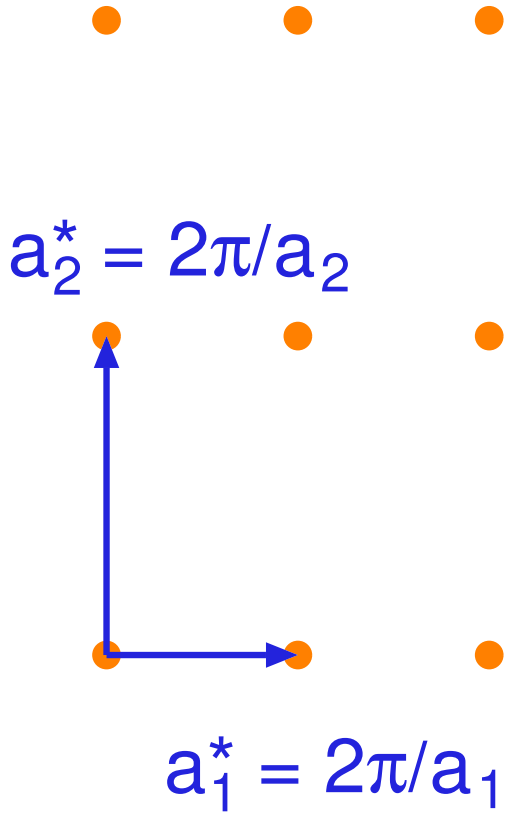

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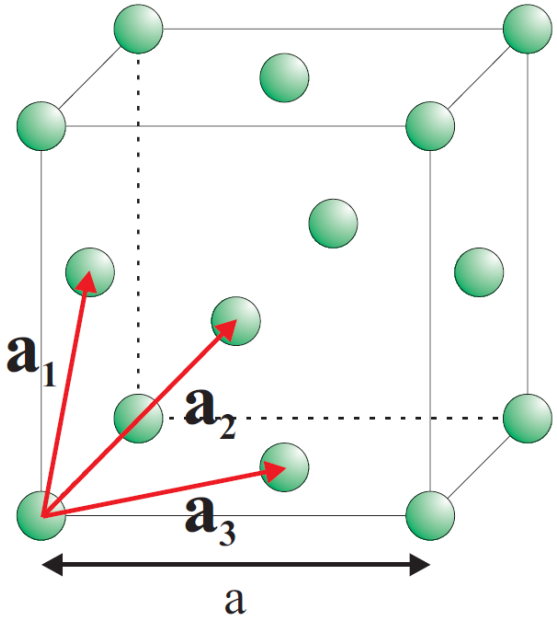
$$= 2\pi(hn_1 + kn_2 + ln_3) = 2\pi m$$

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

The FCC reciprocal lattice

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



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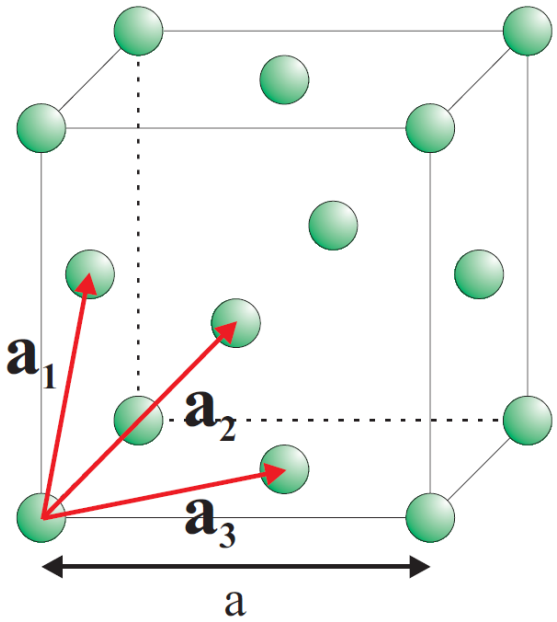

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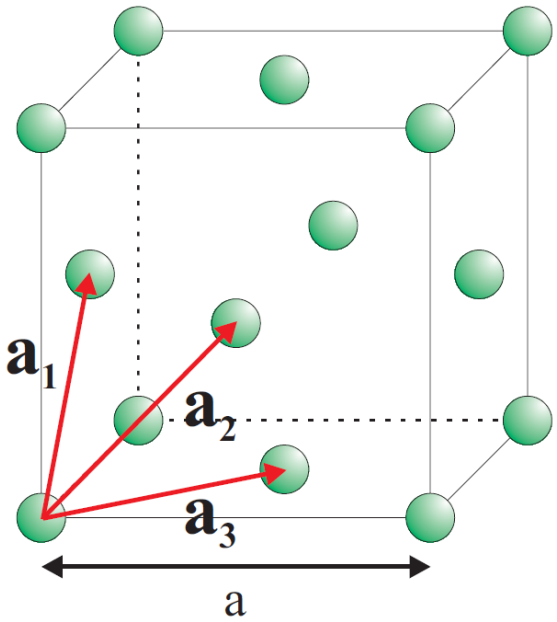

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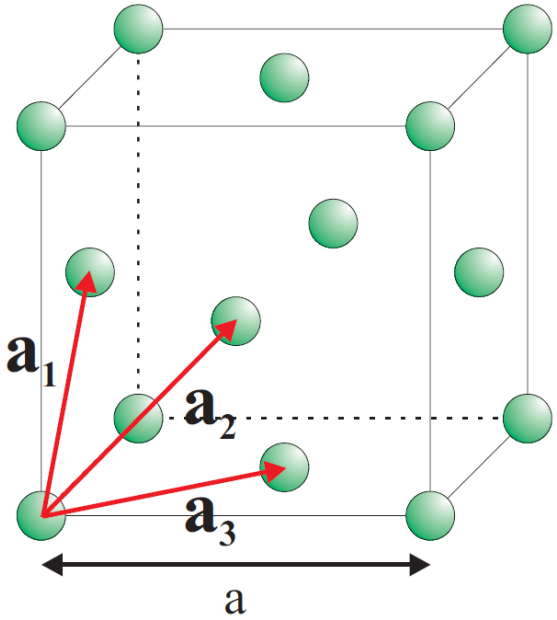

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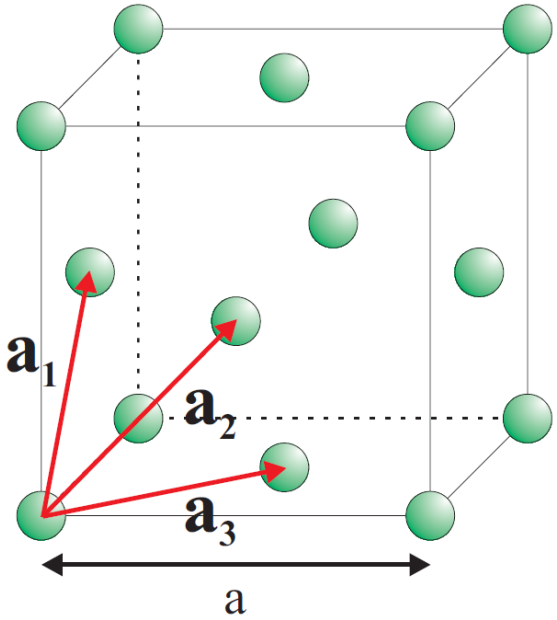

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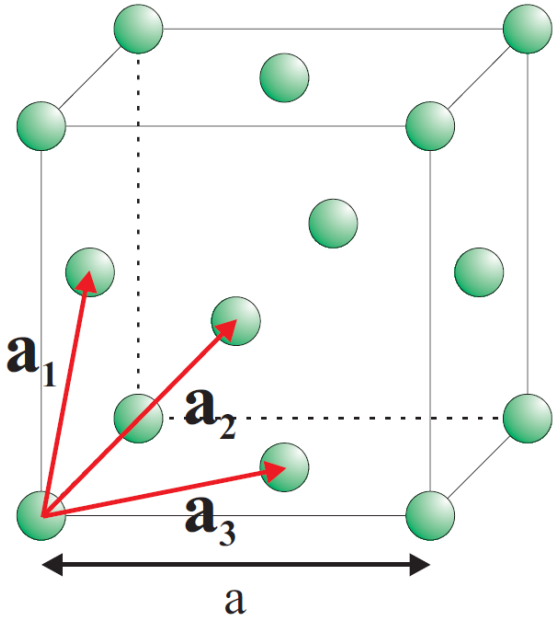

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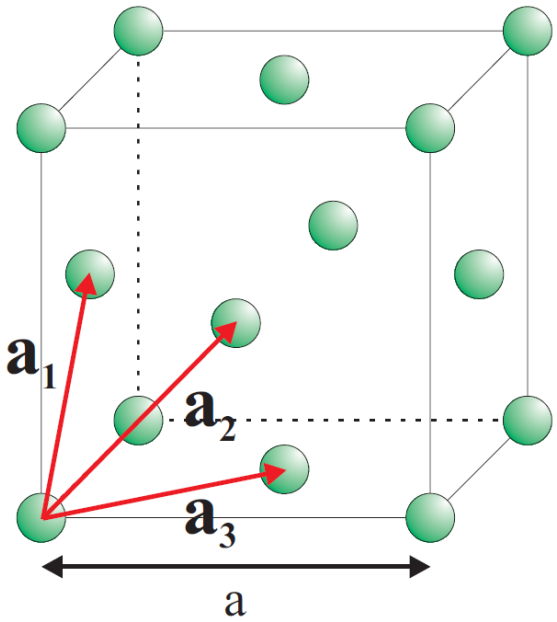

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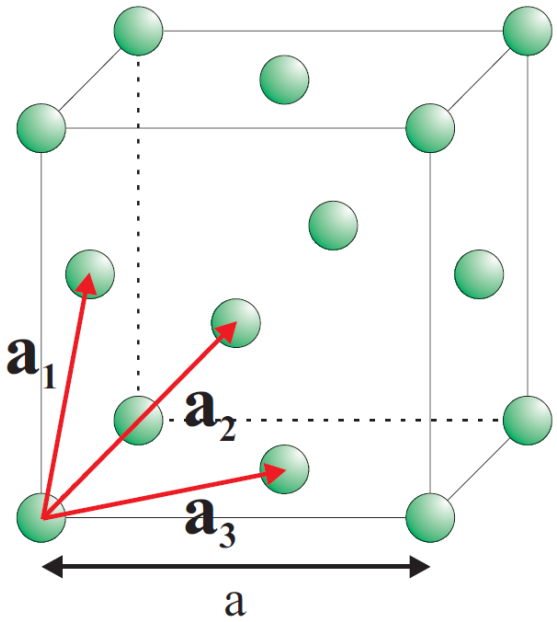

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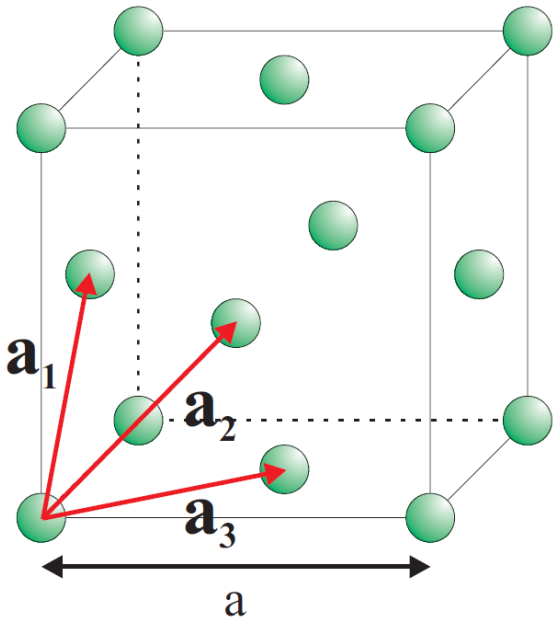

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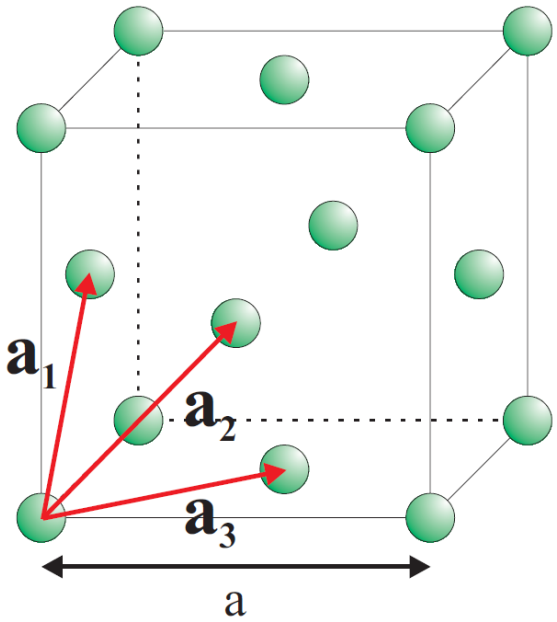

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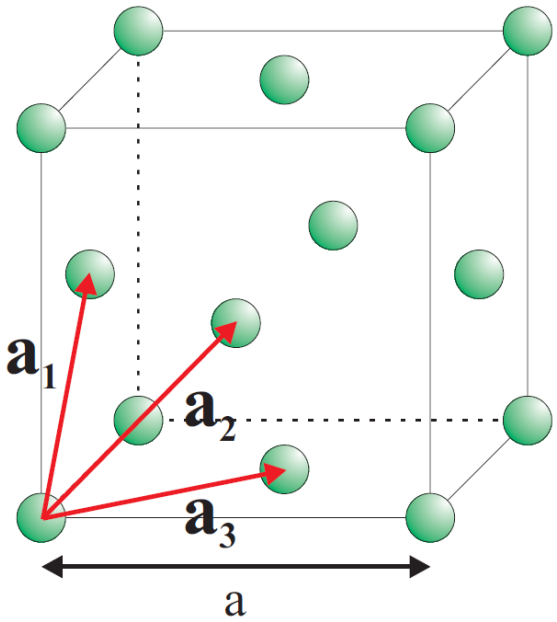

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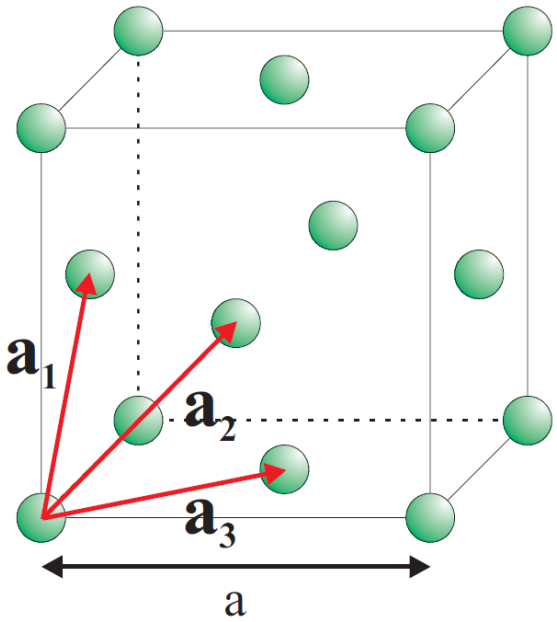

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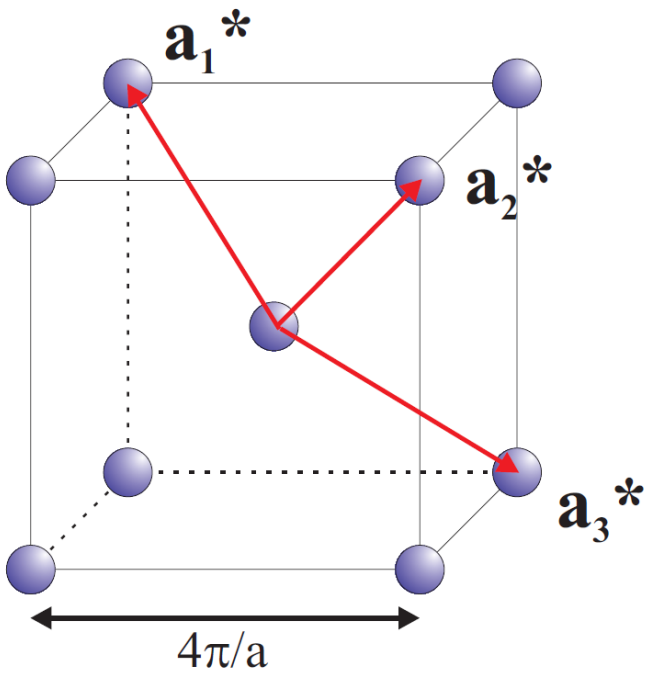

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That is, the lattice sum (scattering factor) is simply proportional to the reciprocal space lattice

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in 2D, with $N_1 \times N_2 = N$ unit cells

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$$= NA^* \sum_{\vec{G}} \delta(\vec{Q} - \vec{G}_h)$$

and similarly in 3D

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

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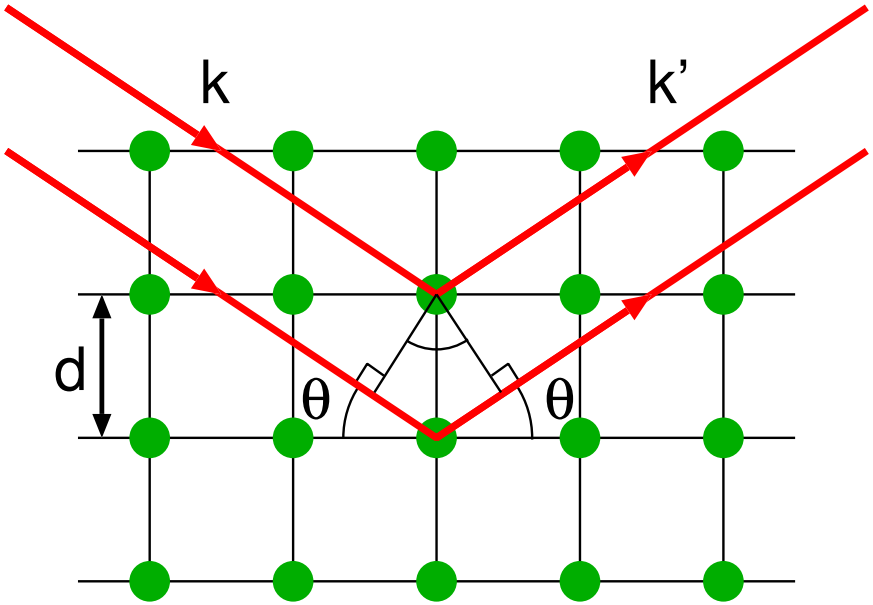
in general

$$\int_{-\infty}^{\infty} \mathcal{L}(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} dV = V_c^* \sum_{h,k,l} \delta(\vec{Q} - \vec{G}_{hkl})$$

Bragg condition



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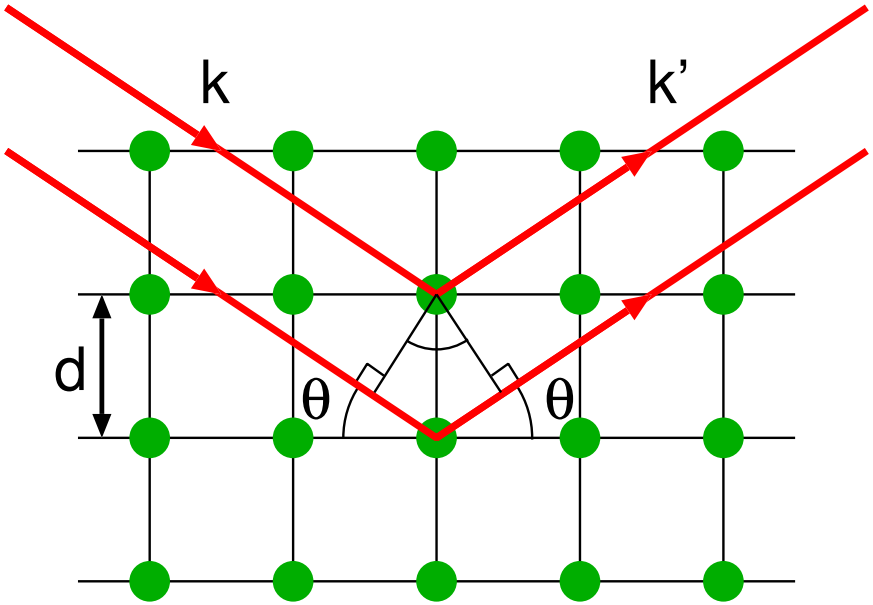

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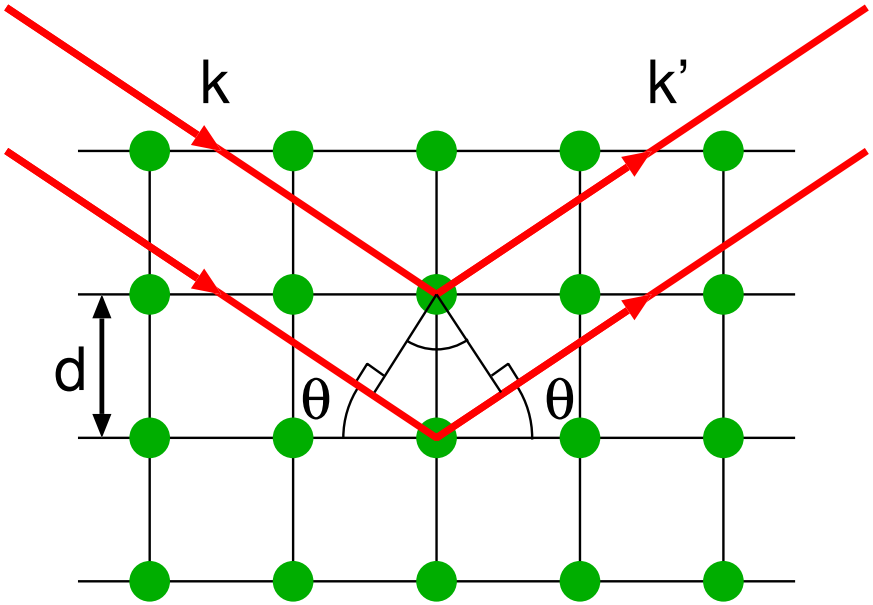

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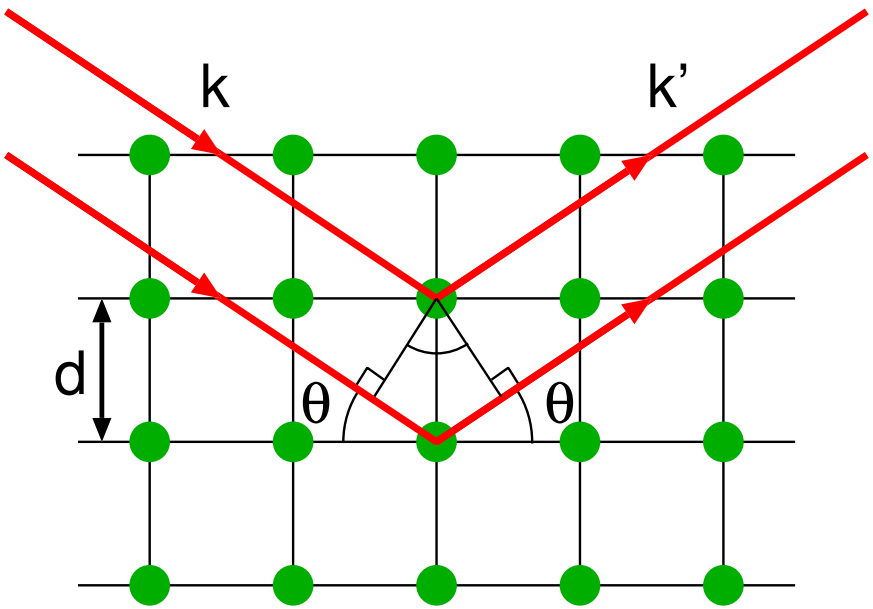

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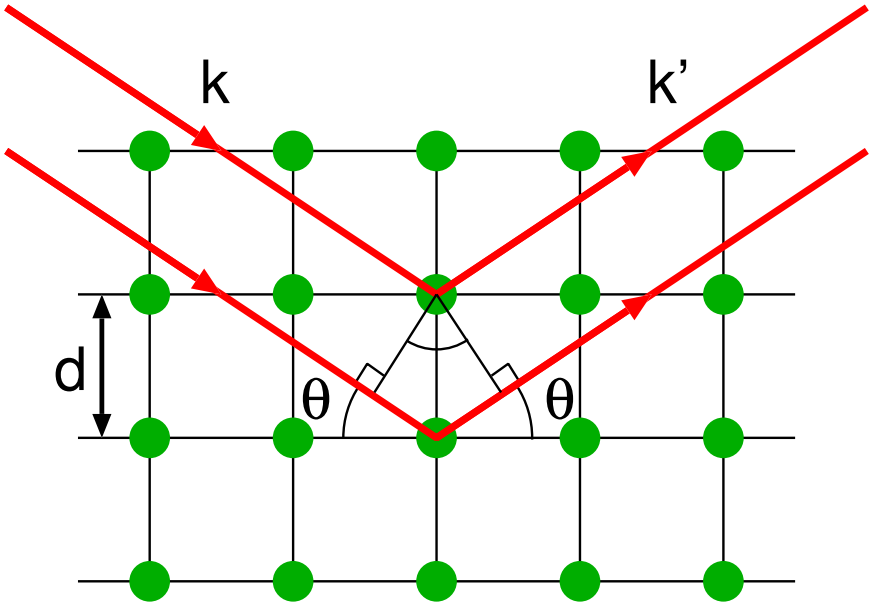

$$2d \sin\theta = \lambda$$

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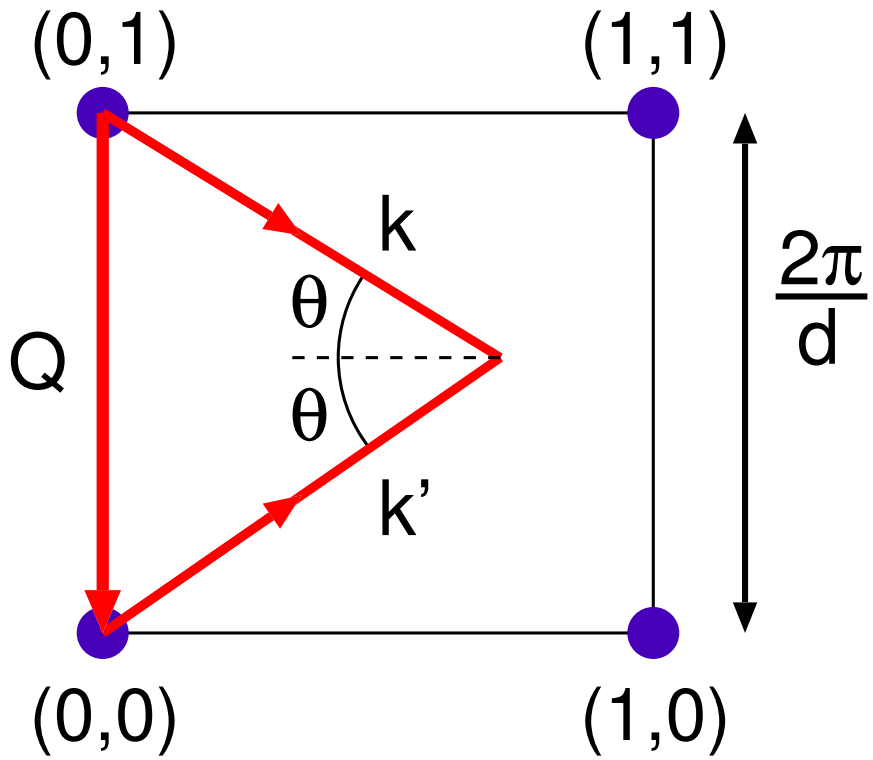
Laue condition

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



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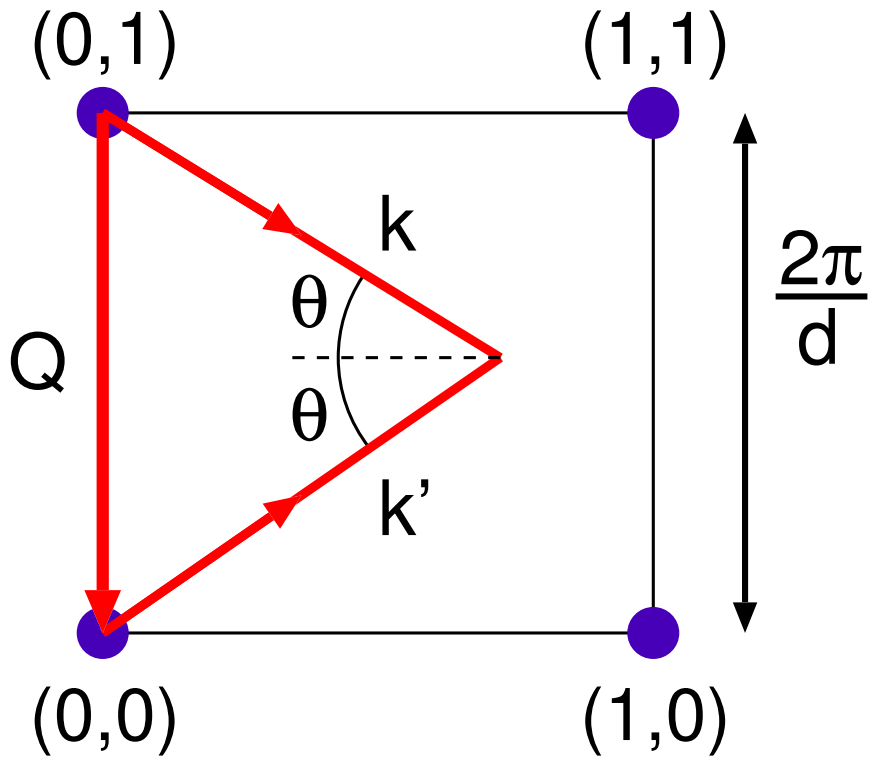

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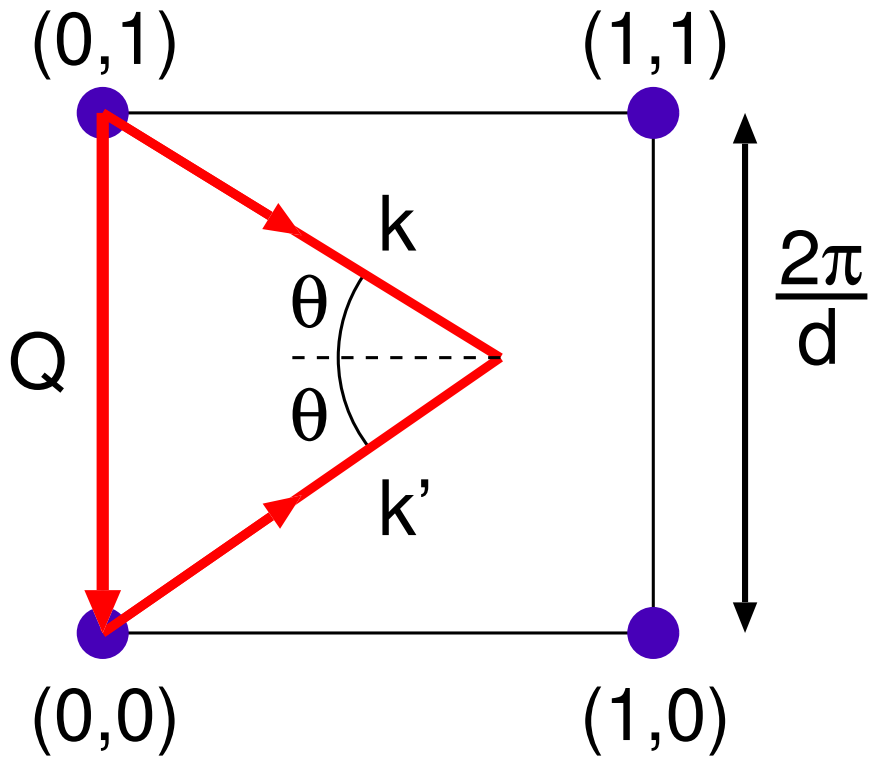

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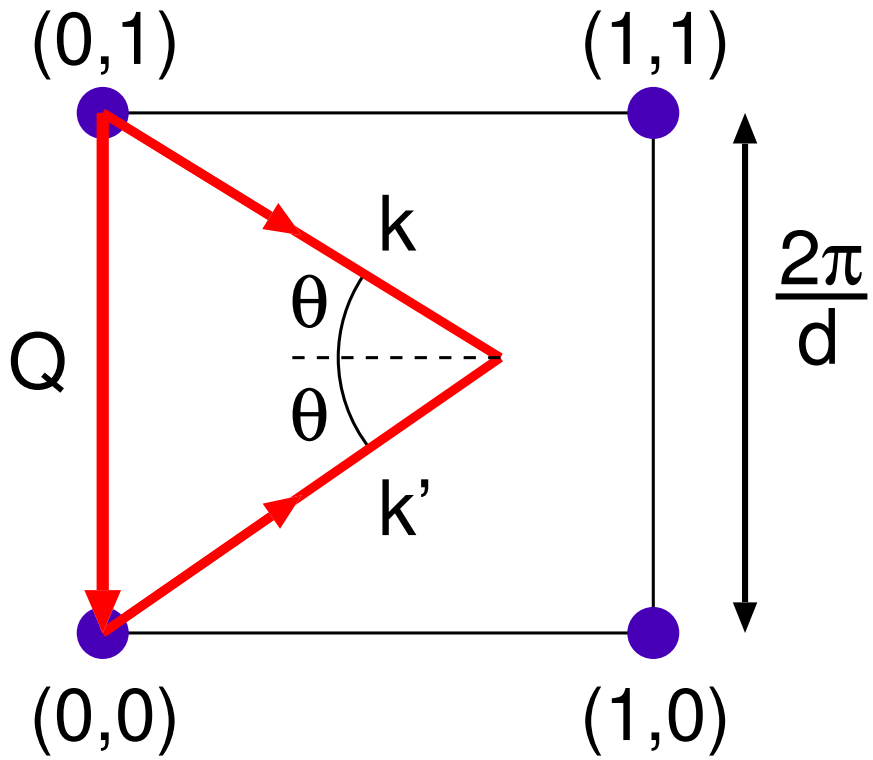

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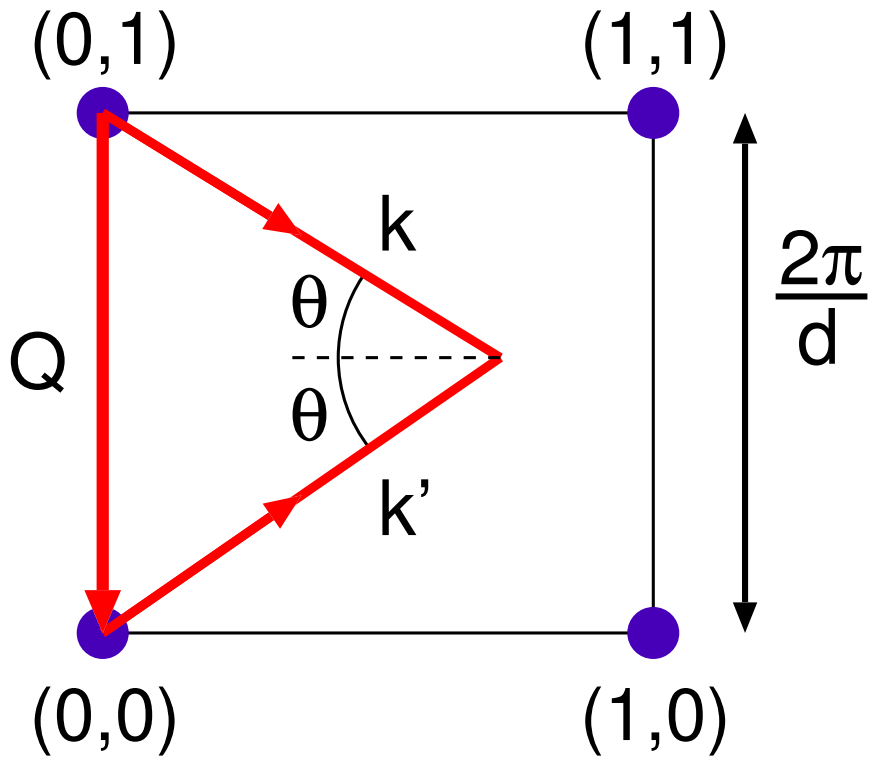

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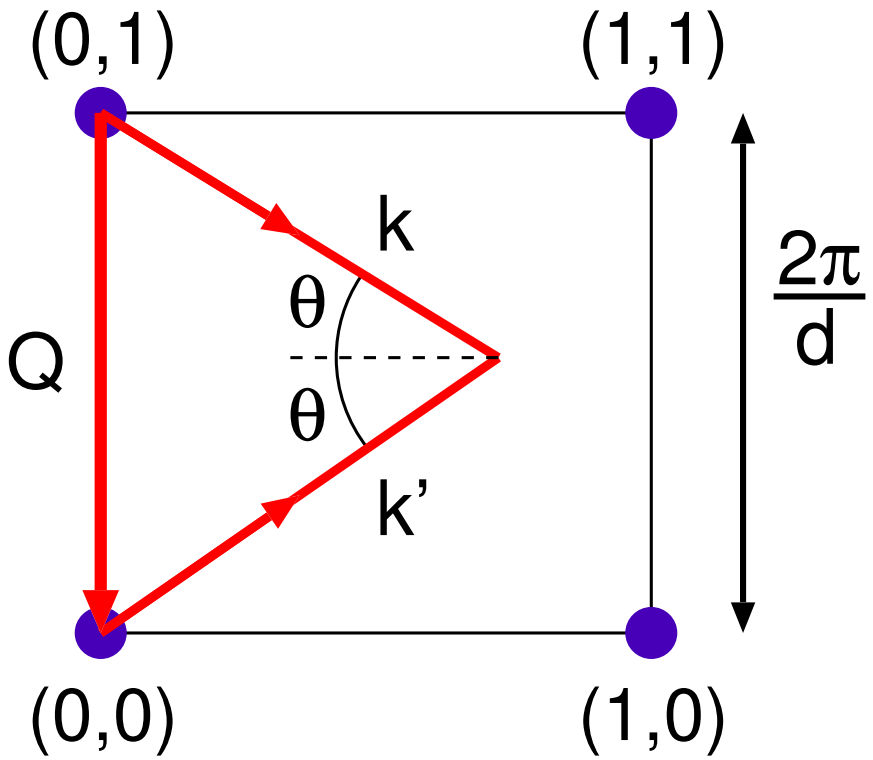

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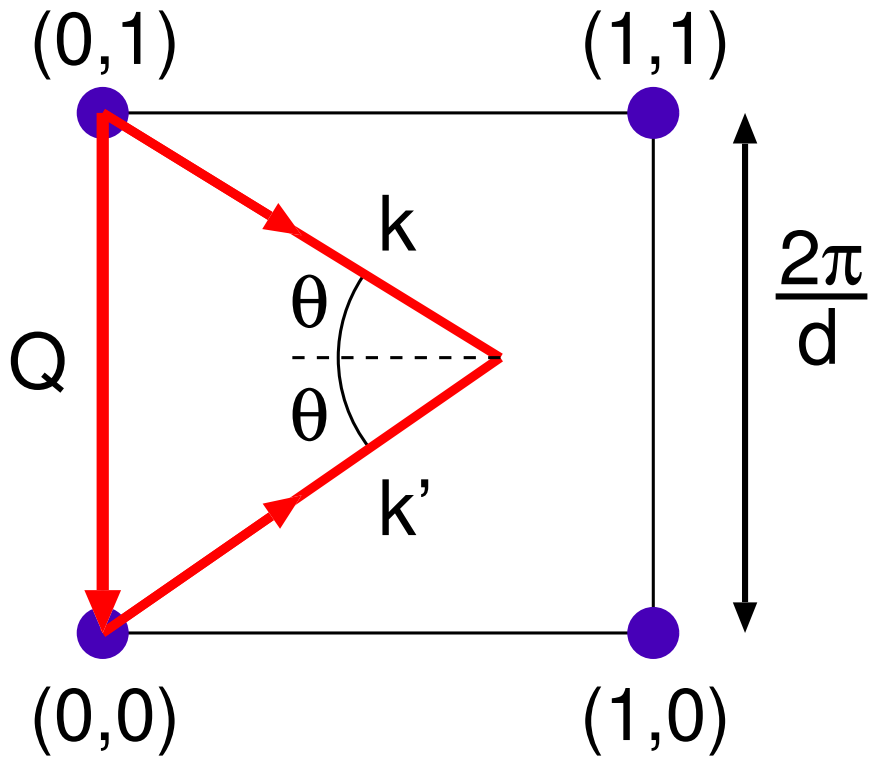

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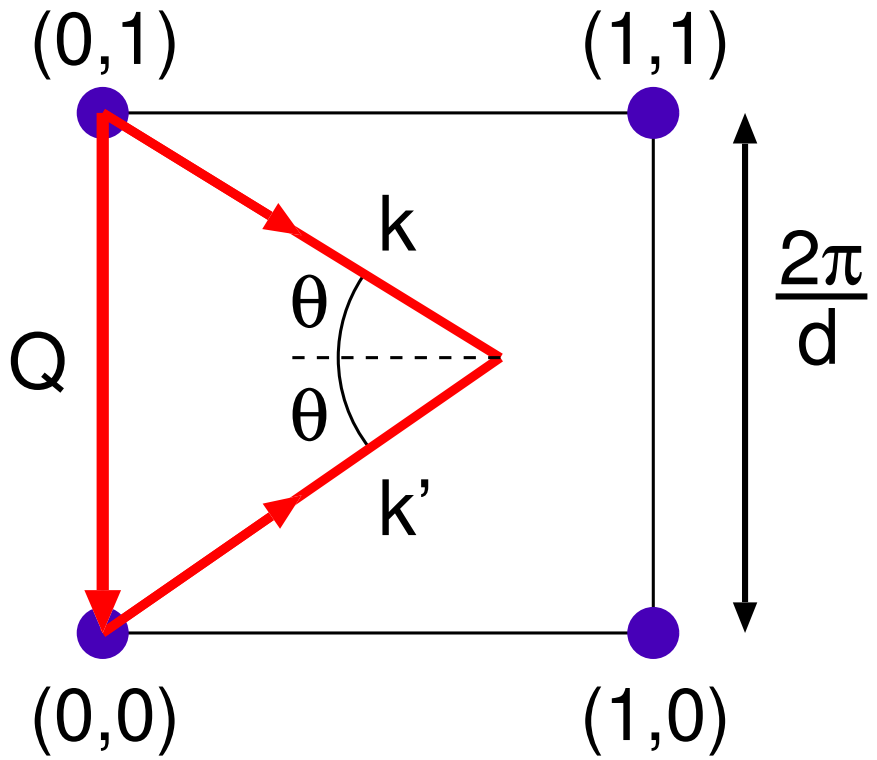
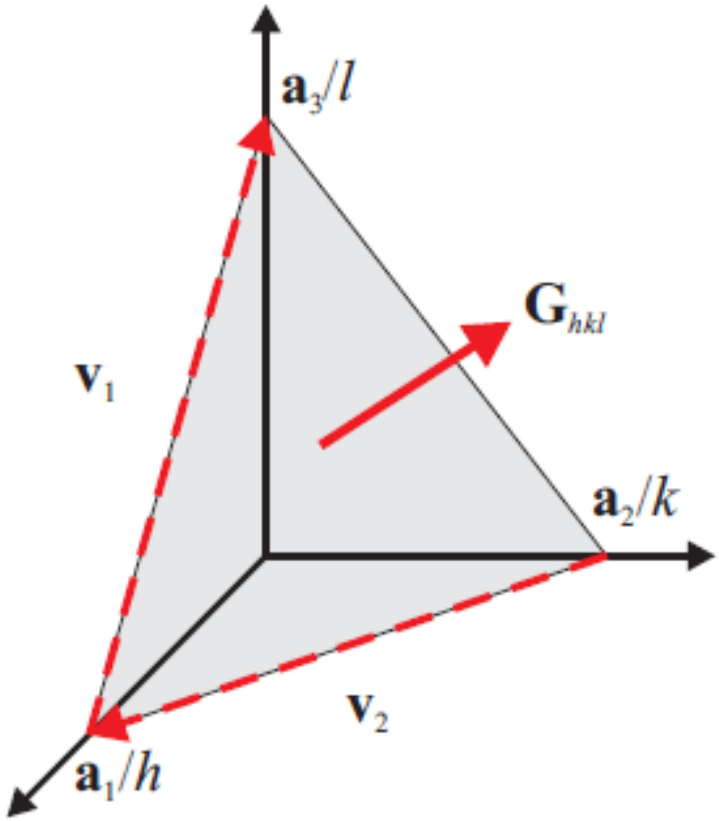


Thus the Bragg and Laue conditions are equivalent

General proof of Bragg-Laue equivalence



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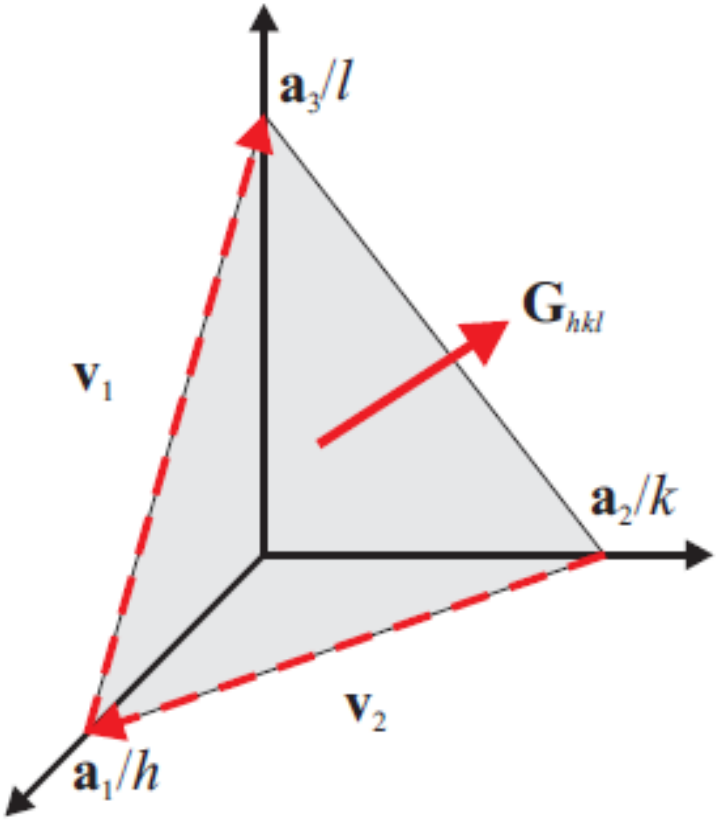

Must show that for each point in reciprocal space, there exists a set of planes in the real space lattice such that:

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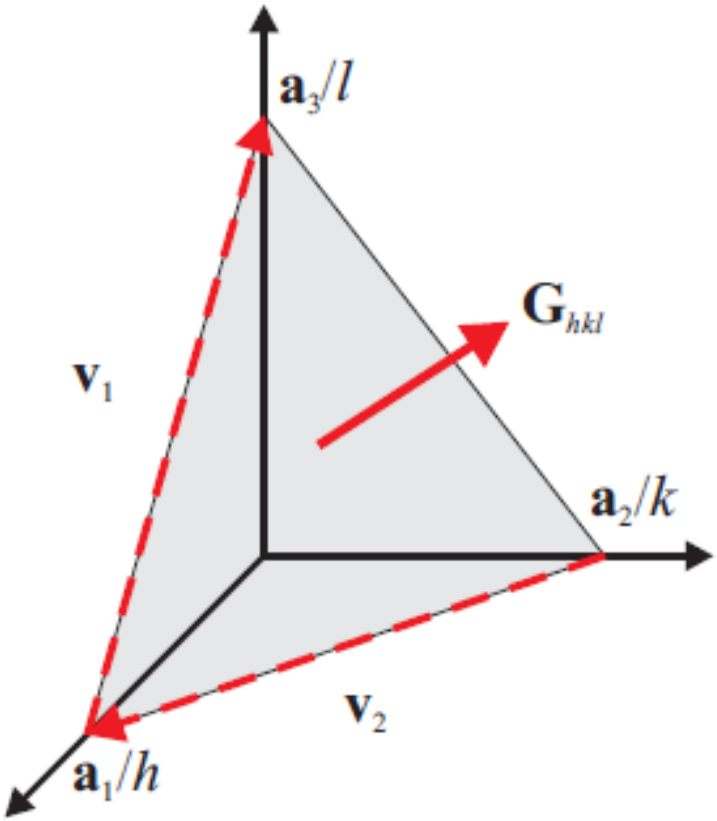

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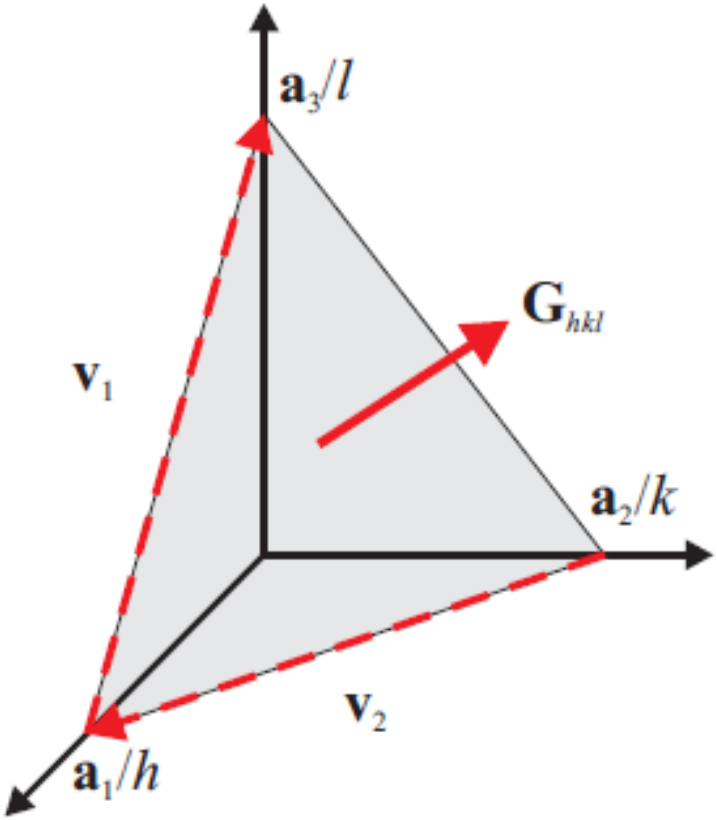

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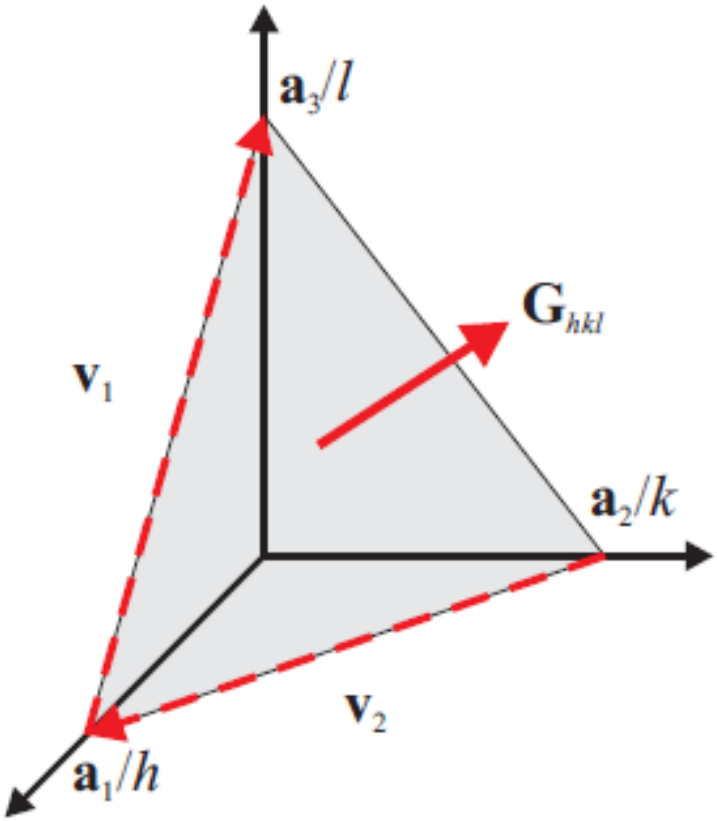

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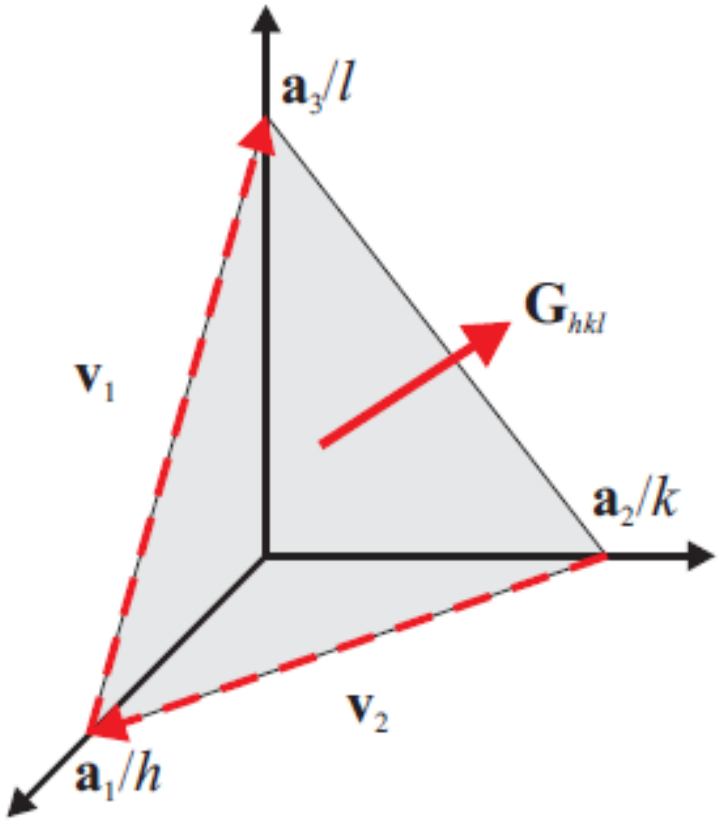

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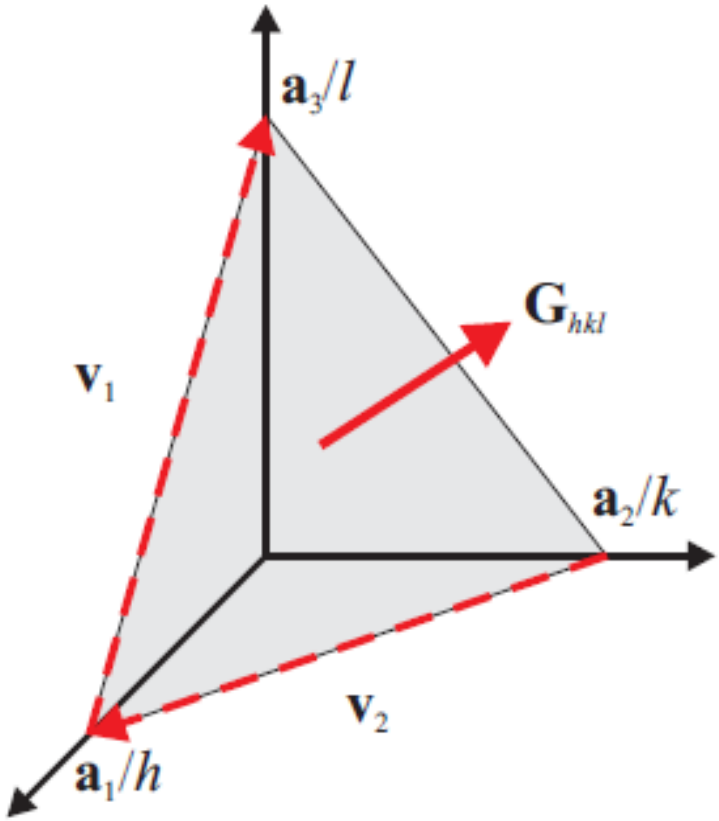

The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

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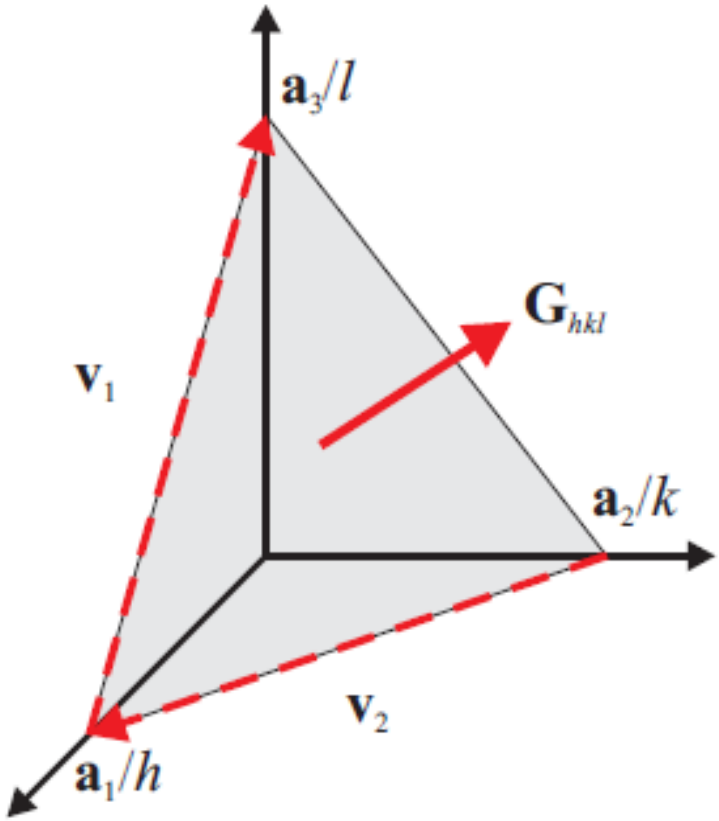

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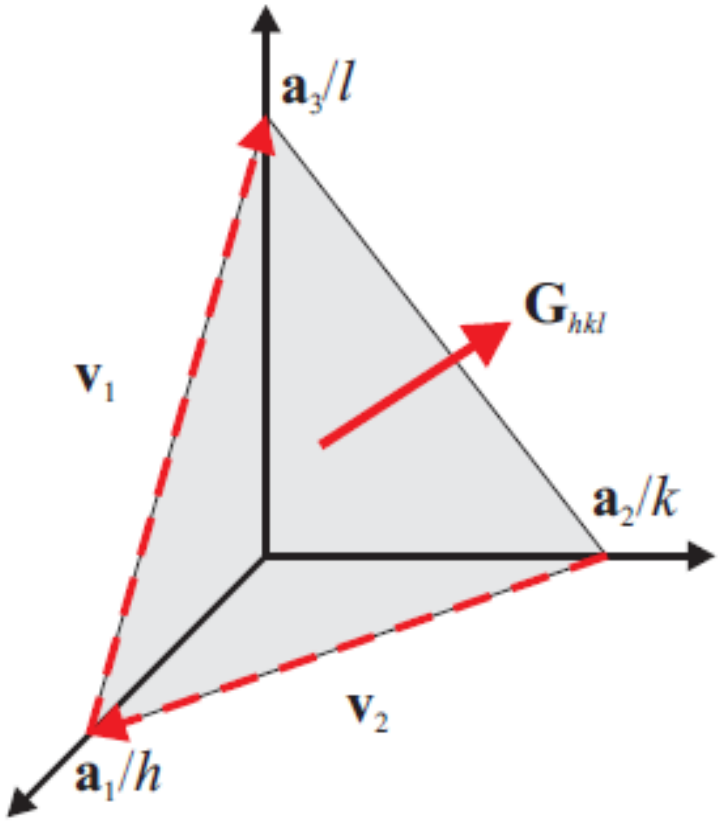

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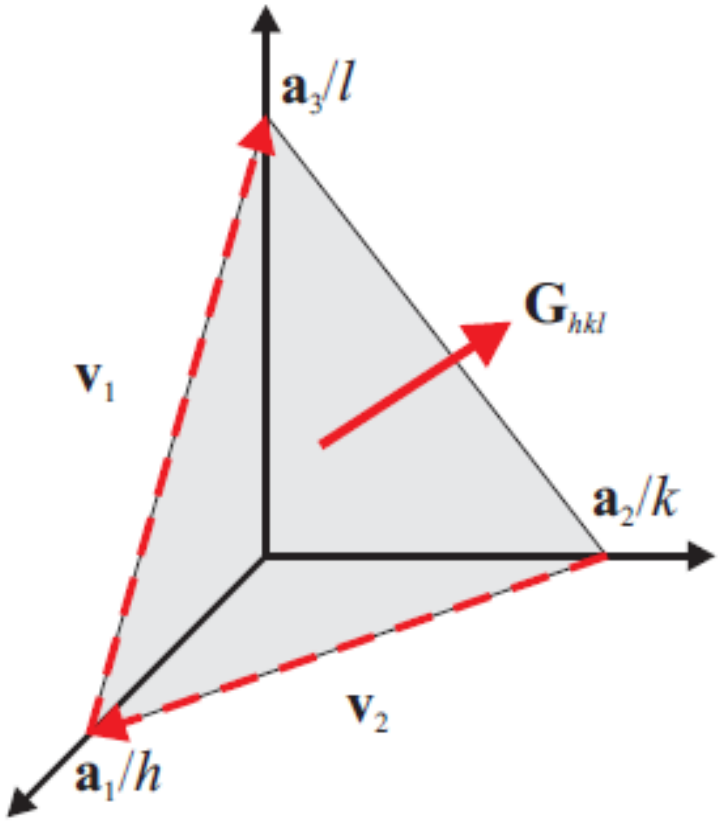

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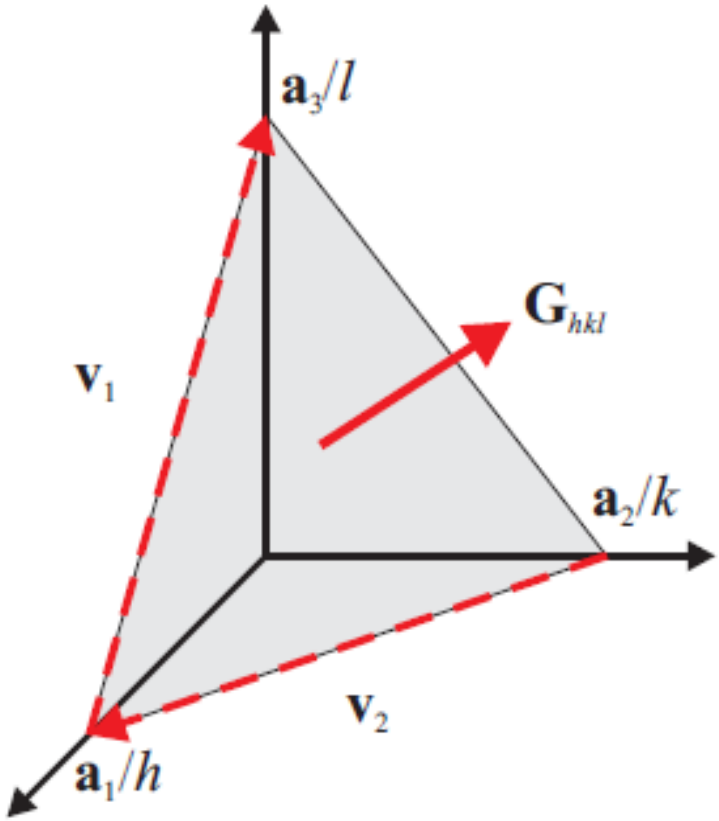

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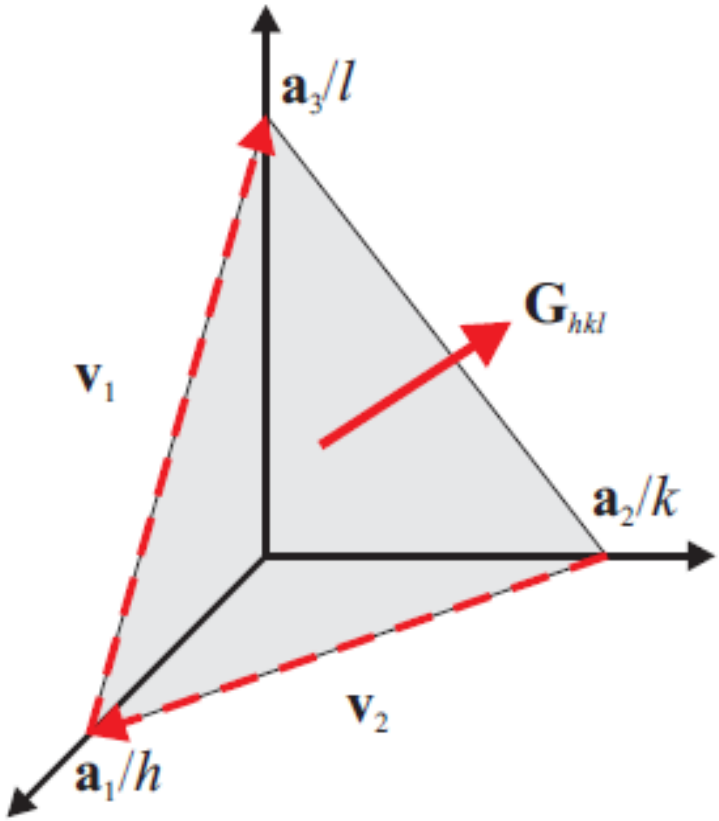

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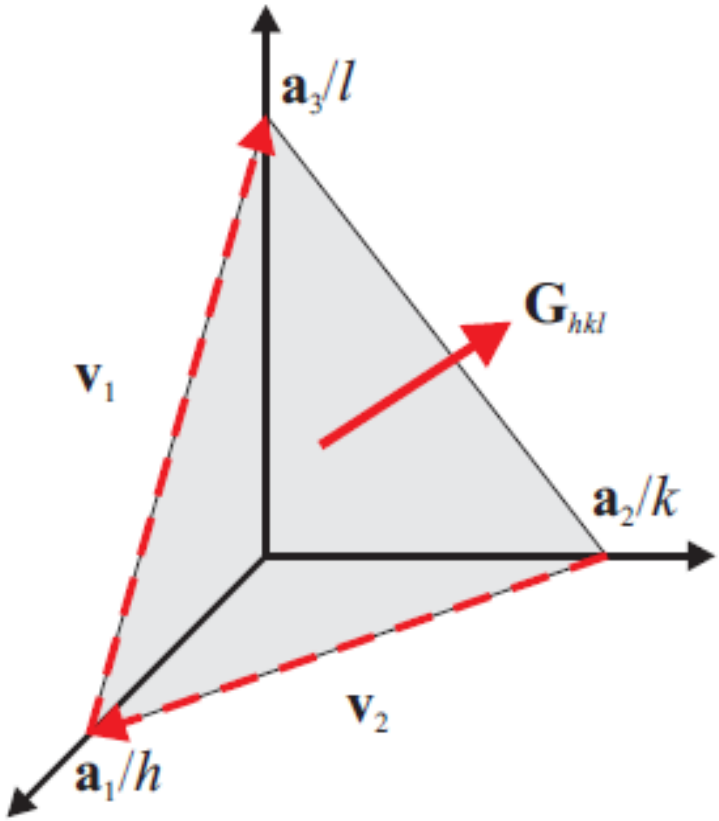

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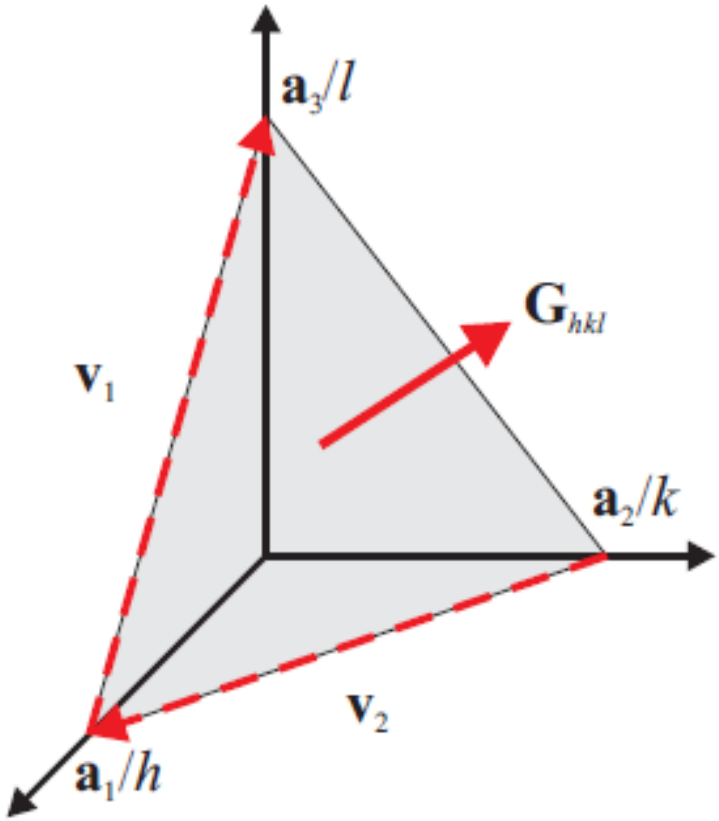

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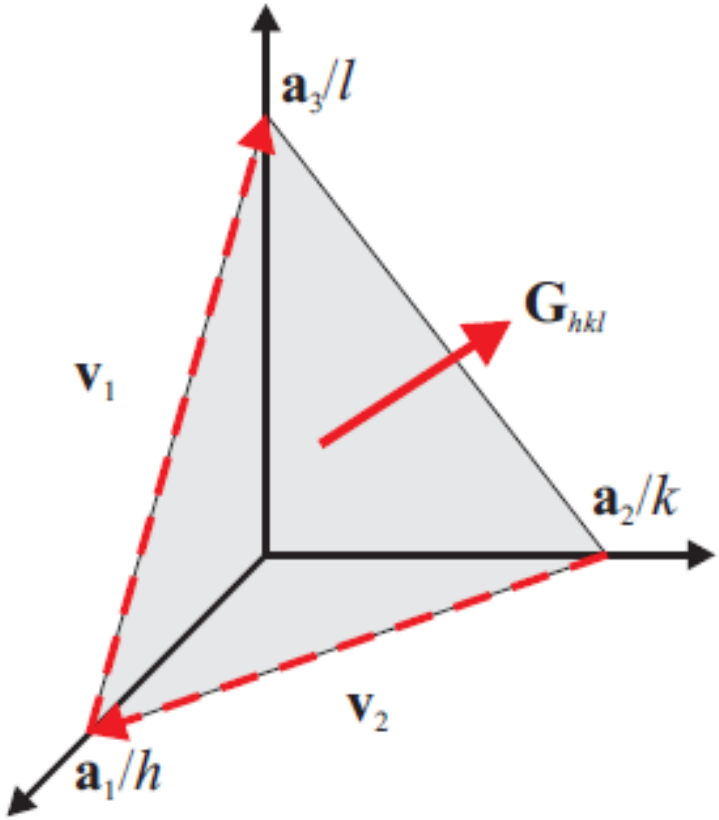
Thus $\vec{G}_{hkl}$ is indeed normal to the plane with Miller indices (hkl)

General proof of Bragg-Laue equivalence



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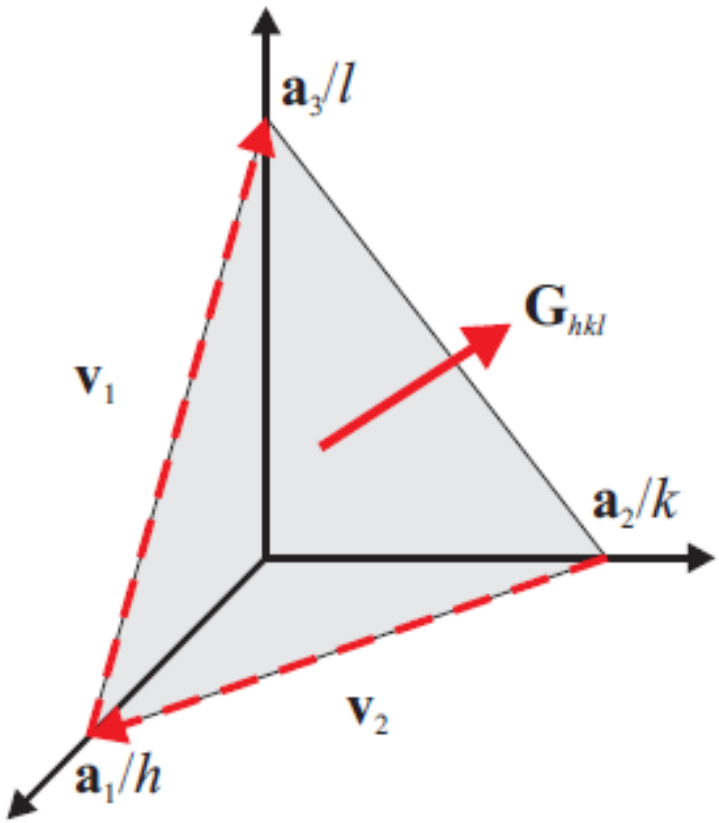
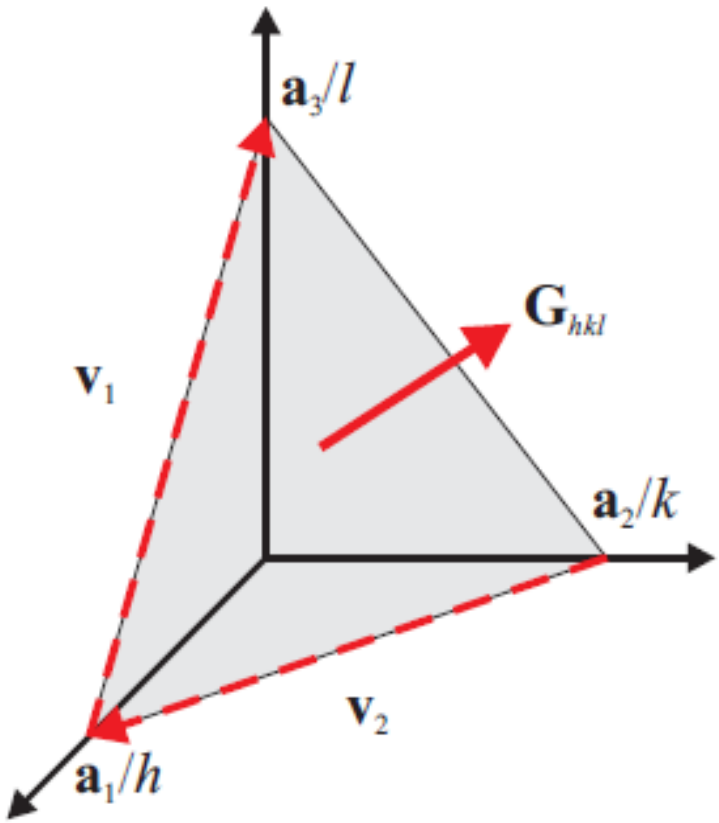


The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

General proof of Bragg-Laue equivalence



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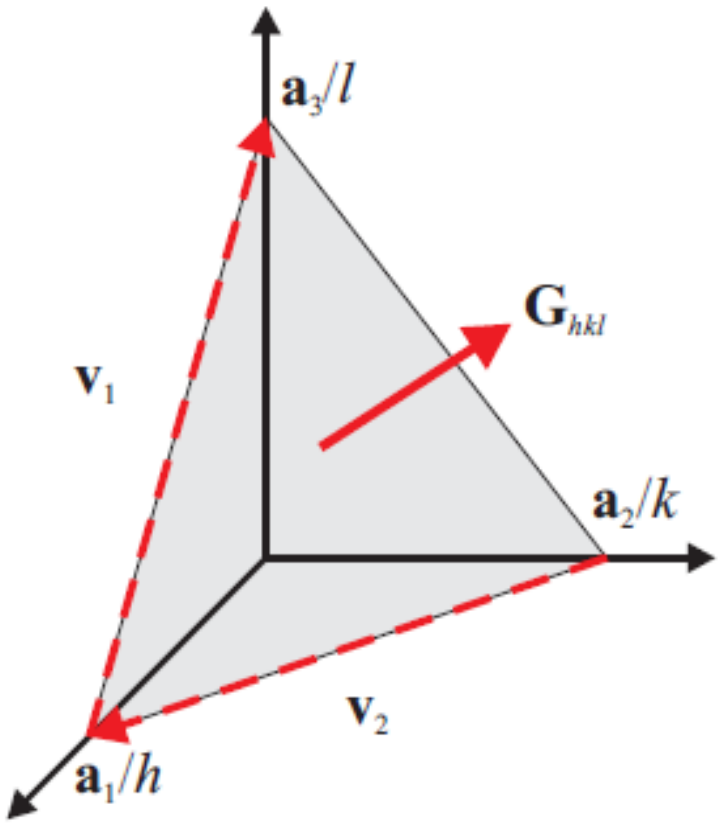

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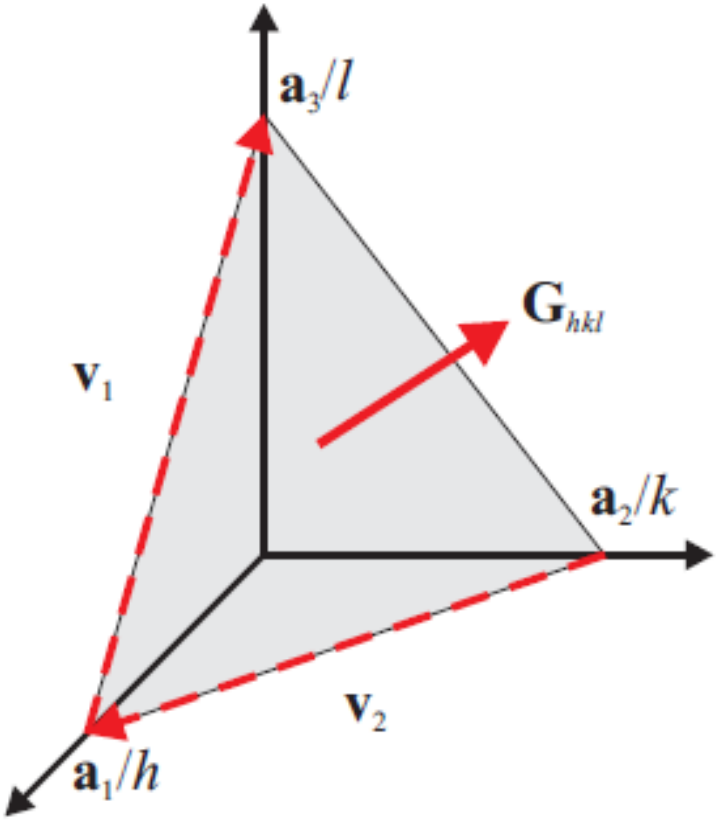

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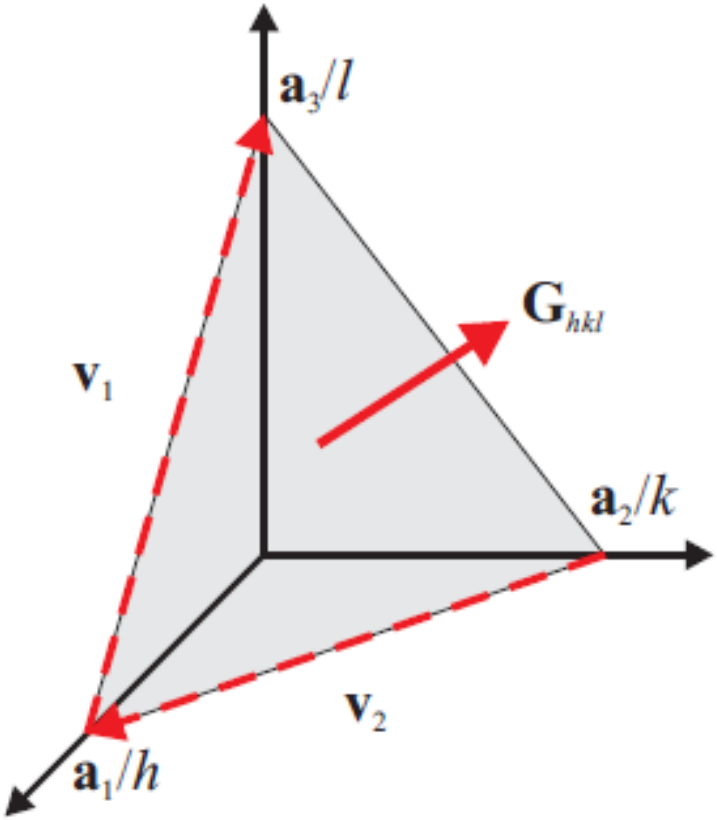
$$\hat{G}_{hkl} \cdot \frac{\vec{a}_1}{h} = \frac{(h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*)}{|\vec{G}_{hkl}|} \cdot \frac{\vec{a}_1}{h}$$

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

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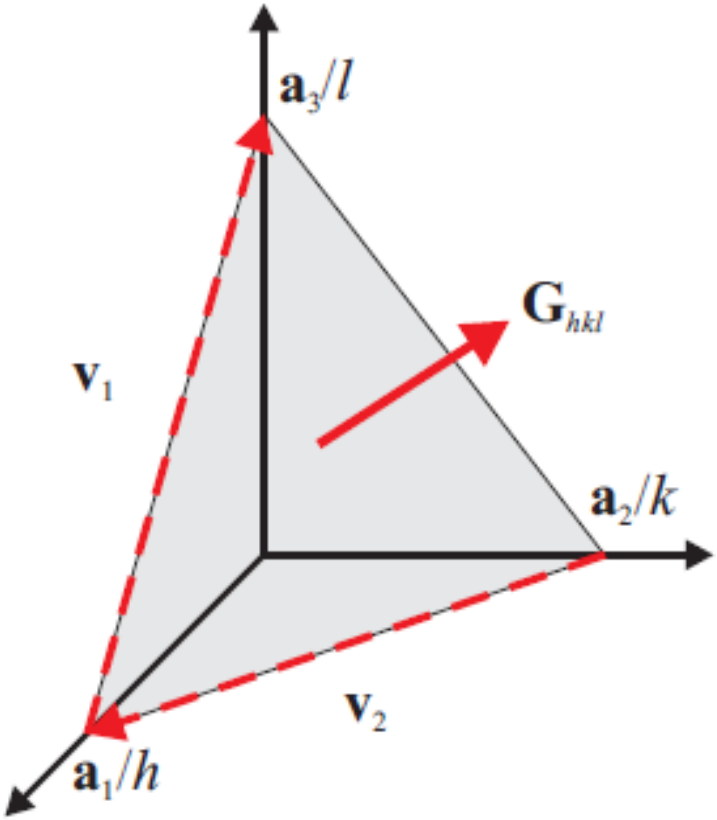

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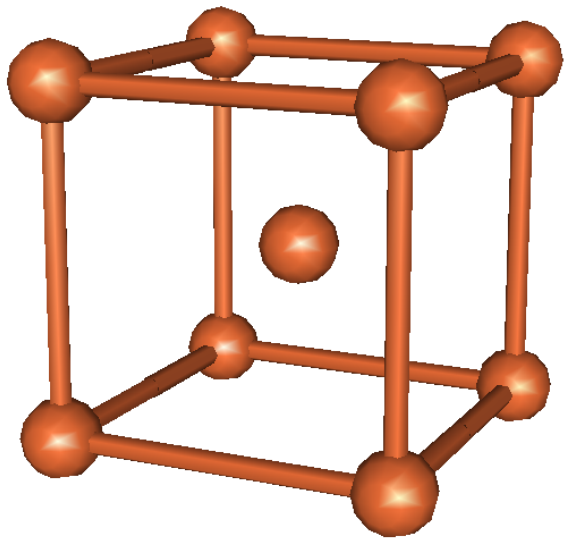
BCC structure factor

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



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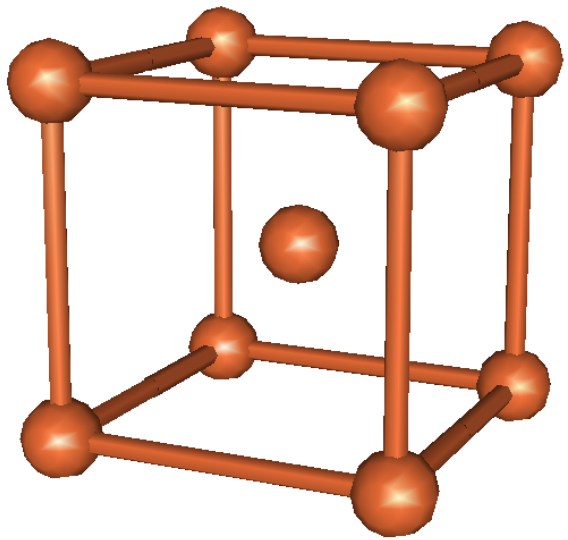

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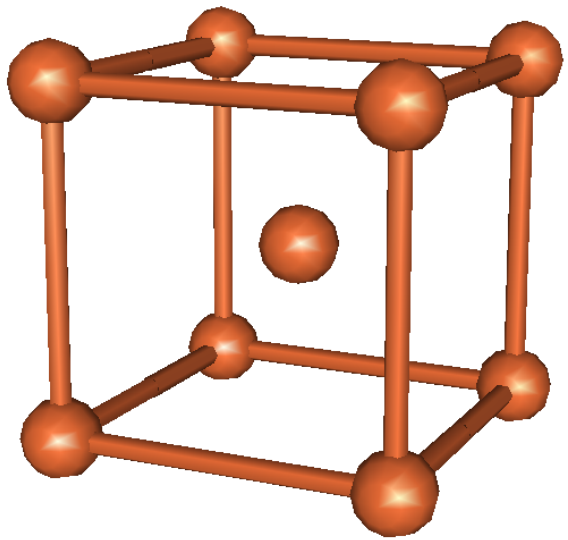

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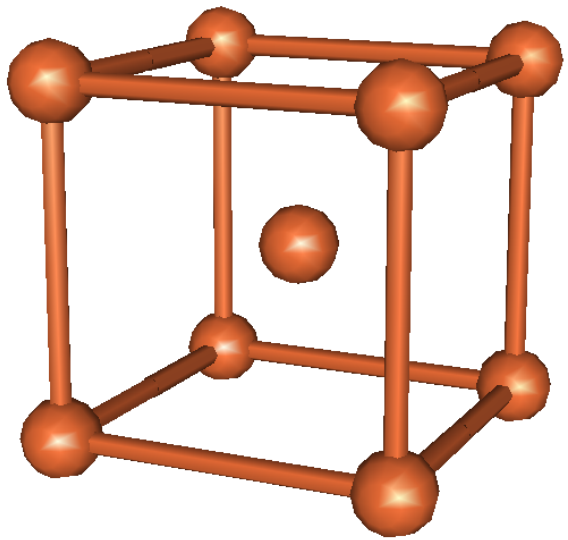

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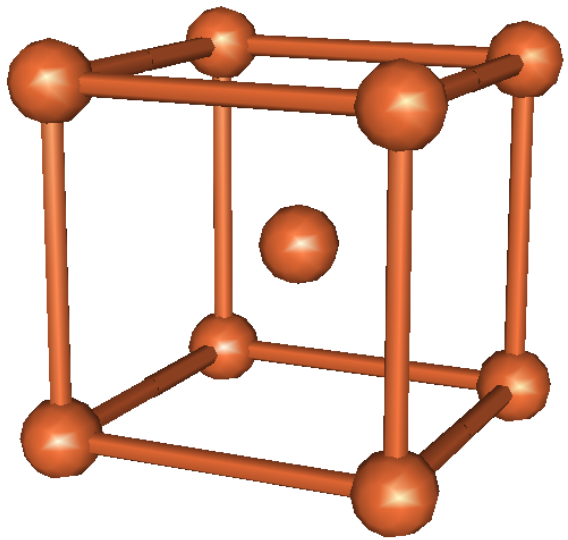
$$\begin{aligned} F_{hkl}^{bcc} &= f(\vec{G}) \sum_j e^{i\vec{G}\cdot\vec{r}_j} \\ &= f(\vec{G}) \left(1 + e^{i\pi(h+k+l)}\right) \end{aligned}$$



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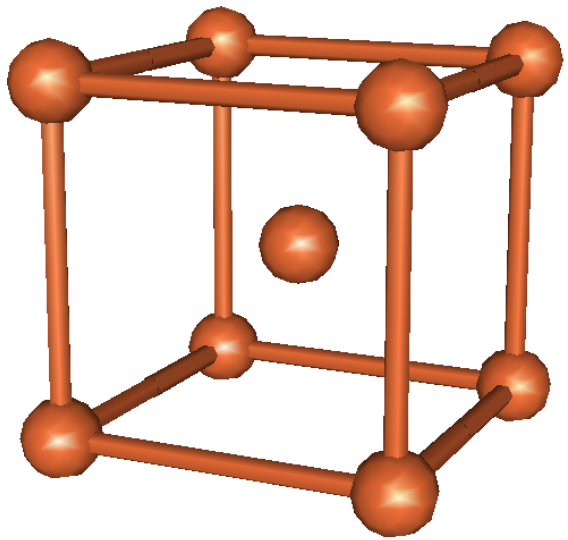
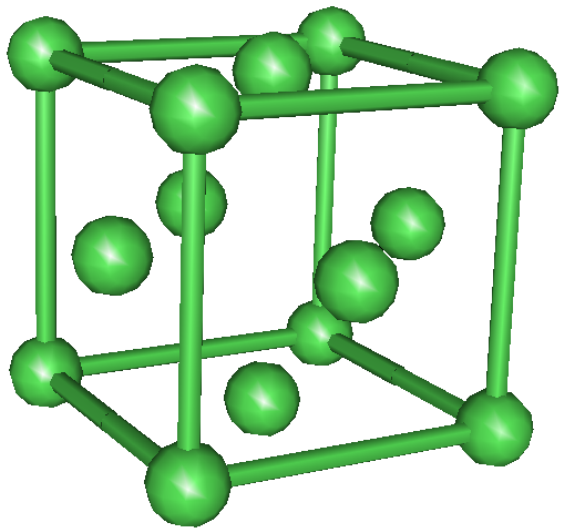


FCC structure factor

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



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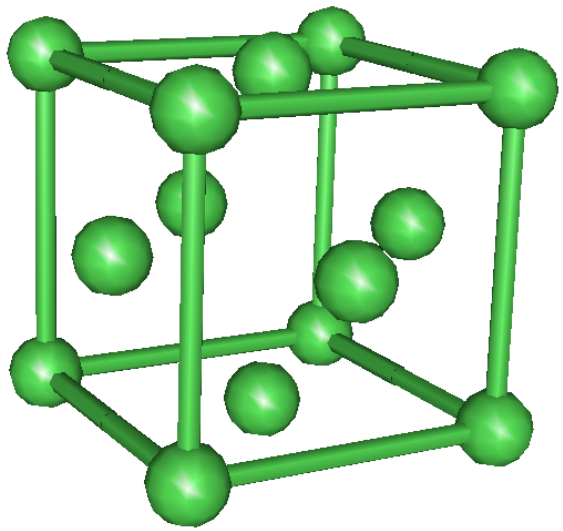

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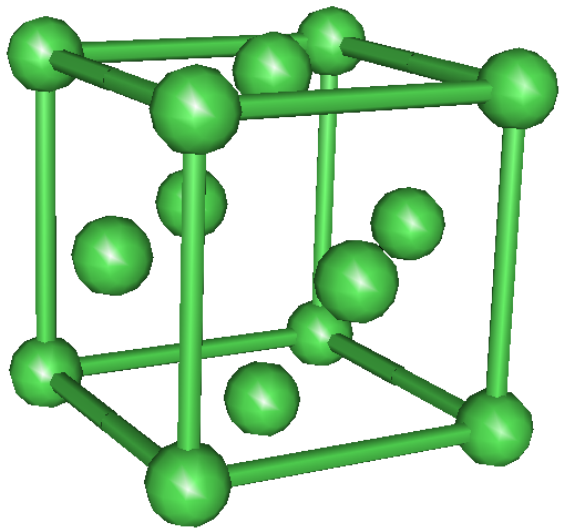

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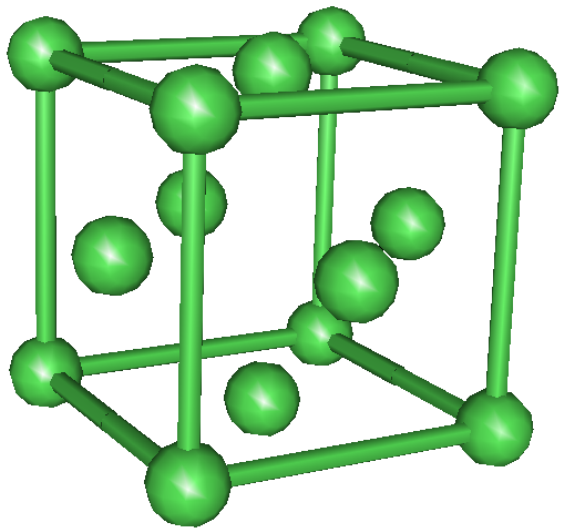

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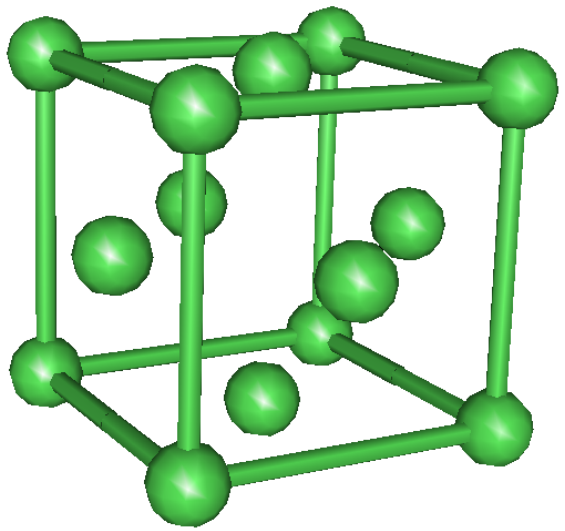
$$= f(\vec{G}) \left(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)}\right)$$



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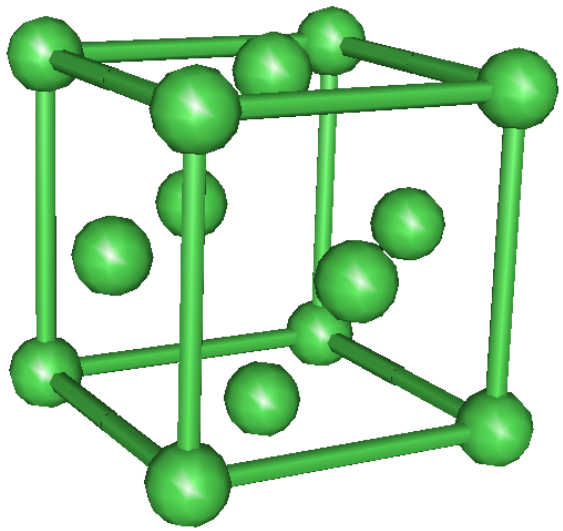
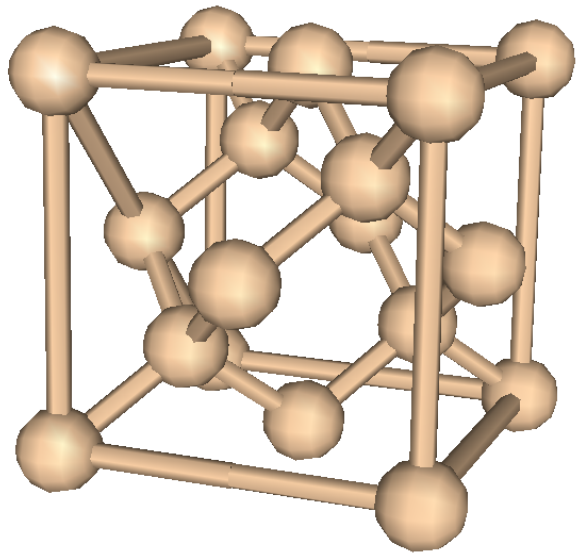


Diamond structure

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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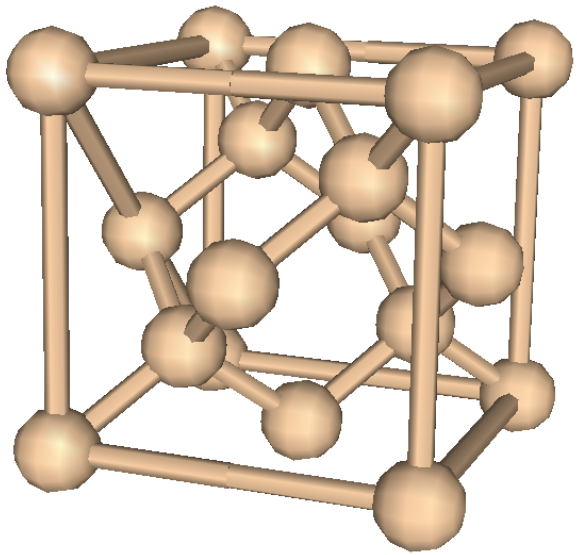
$$\vec{r}_5 = \frac{1}{4}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3), \quad \vec{r}_6 = \frac{1}{4}(3\vec{a}_1 + 3\vec{a}_2 + \vec{a}_3)$$

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



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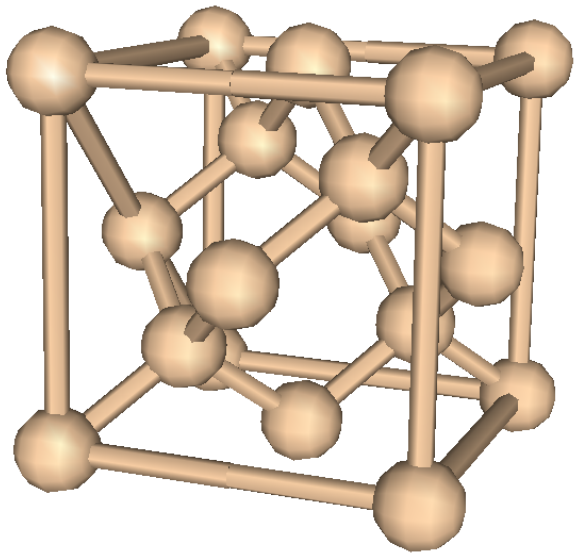
$$F_{hkl}^{diamond} = f(\vec{G})\Big(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k+l)/2} + e^{i\pi(3h+3k+l)/2} + e^{i\pi(h+3k+3l)/2} + e^{i\pi(3h+k+3l)/2}\Big)$$



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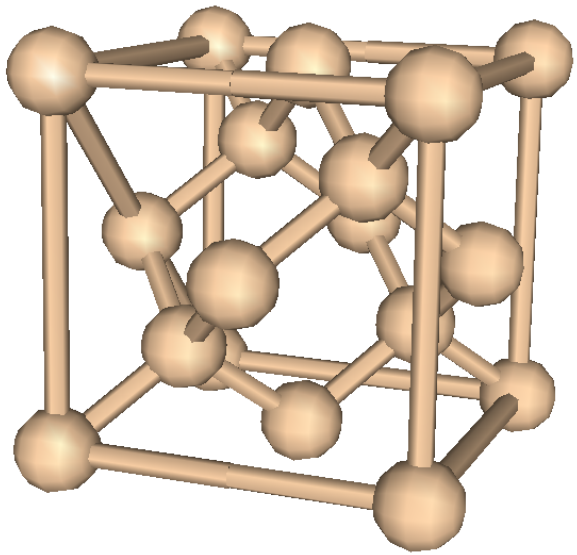
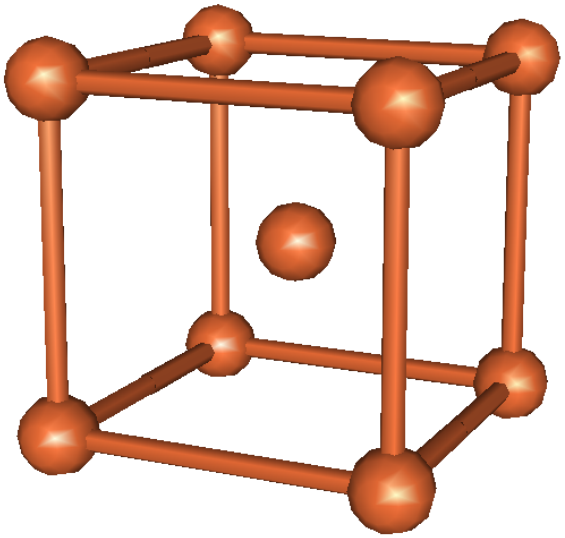


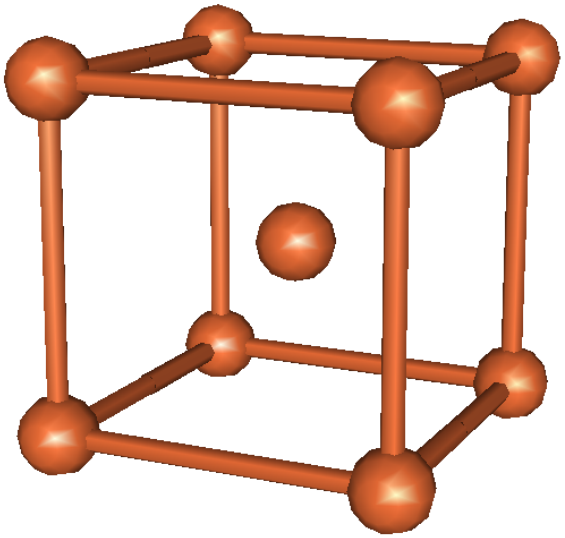
This is non-zero when h,k,l all even and $h + k + l = 4n$ or h,k,l all odd

Heteroatomic structures



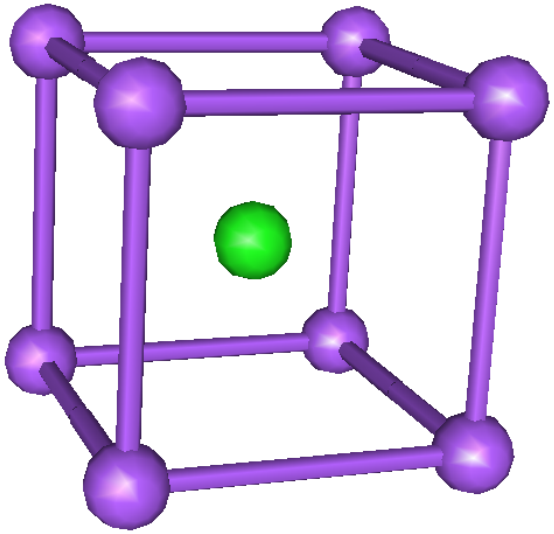
← bcc

Heteroatomic structures



← bcc

sc →



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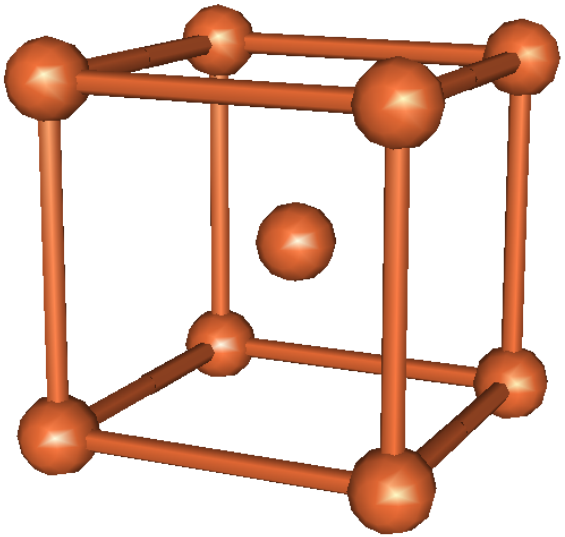

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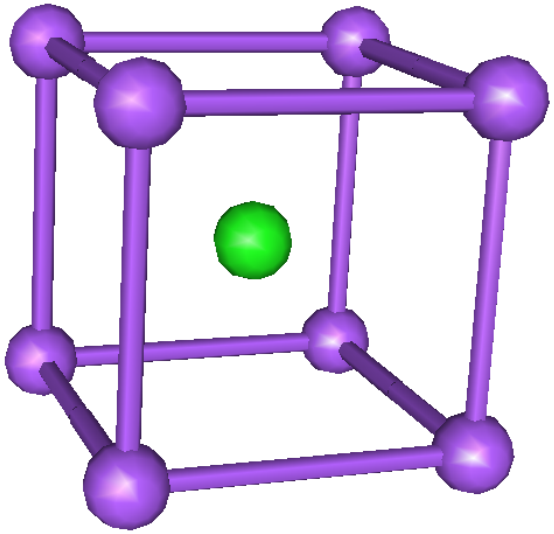
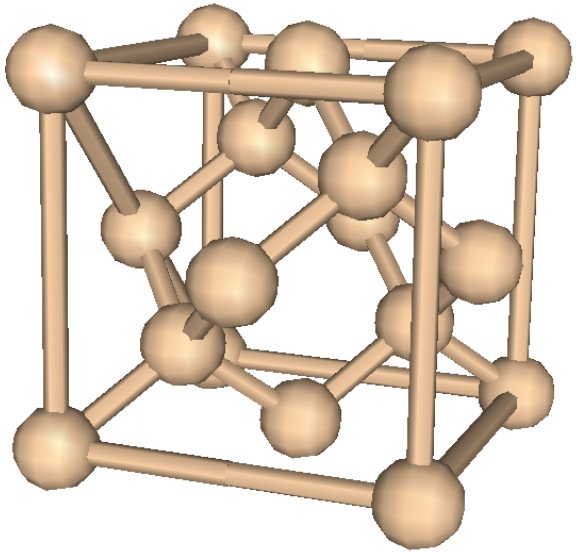
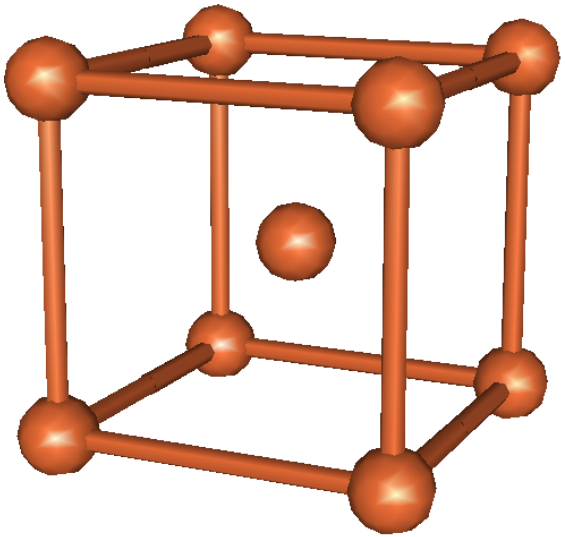




← diamond

Heteroatomic structures



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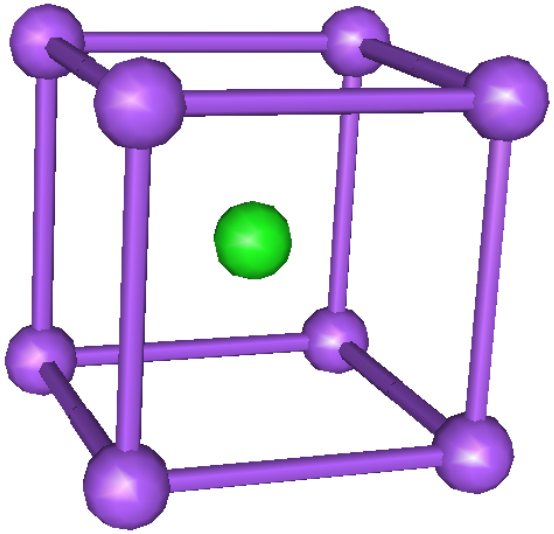
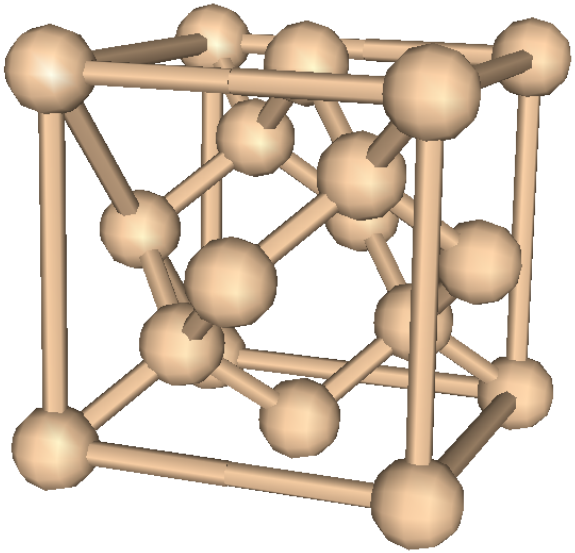
sc →





← diamond

fcc →