Today's Outline - October 17, 2016

Today's Outline - October 17, 2016

- Final project

Today's Outline - October 17, 2016

- Final project
- Structure factors

Today's Outline - October 17, 2016

- Final project
- Structure factors
- Ewald construction

Today's Outline - October 17, 2016

- Final project
- Structure factors
- Ewald construction
- Incommensurate crystals

Today's Outline - October 17, 2016

- Final project
- Structure factors
- Ewald construction
- Incommensurate crystals

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

Final project

1. Come up with a potential experiment

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation
3. Clear it with me!

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation
3. Clear it with me!
4. Find appropriate beamline(s) and if needed contact the beamline scientists (they are used to it)

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation
3. Clear it with me!
4. Find appropriate beamline(s) and if needed contact the beamline scientists (they are used to it)
5. Lay out proposed experiment (you can ask for help!)

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation
3. Clear it with me!
4. Find appropriate beamline(s) and if needed contact the beamline scientists (they are used to it)
5. Lay out proposed experiment (you can ask for help!)
6. Make sure to give reasonable answers forall the questions

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation
3. Clear it with me!
4. Find appropriate beamline(s) and if needed contact the beamline scientists (they are used to it)
5. Lay out proposed experiment (you can ask for help!)
6. Make sure to give reasonable answers forall the questions
7. Put me as one of the investigators of the proposal

Final project

1. Come up with a potential experiment
2. Make sure it is a different technique than your final presentation
3. Clear it with me!
4. Find appropriate beamline(s) and if needed contact the beamline scientists (they are used to it)
5. Lay out proposed experiment (you can ask for help!)
6. Make sure to give reasonable answers forall the questions
7. Put me as one of the investigators of the proposal
8. Add my graduate students too

   Yujia Ding
   Shankar Aryal
   Nathaniel Beaver
   Kamil Kucuk
   Elahe Moazzen

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$

First evaluate this sum in 1D. $\vec{R}_n = na$, thus for N unit cells

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$
$$= \sum_{n=0}^{N-1} e^{iQna}$$

First evaluate this sum in 1D. $\vec{R}_n = na$, thus for N unit cells

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$

$$= \sum_{n=0}^{N-1} e^{iQna}$$

First evaluate this sum in 1D. $\vec{R}_n = na$, thus for N unit cells

Which has been evaluated previously as

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$

$$= \sum_{n=0}^{N-1} e^{iQna}$$

$$|S_N(Q)| = \frac{\sin(NQa/2)}{\sin(Qa/2)}$$

First evaluate this sum in 1D. $\vec{R}_n = na$, thus for N unit cells

Which has been evaluated previously as

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$

$$= \sum_{n=0}^{N-1} e^{iQna}$$

$$|S_N(Q)| = \frac{\sin(NQa/2)}{\sin(Qa/2)}$$

First evaluate this sum in 1D. $\vec{R}_n = na$, thus for N unit cells

Which has been evaluated previously as and leads to the Laue condition for diffraction. Looking at the regime where the Laue condition is not exactly fulfilled

$$Q = (h+\xi)a^*$$

Lattice sum in 1D

In order to compute the intensity of a specific Bragg reflection, we consider the lattice sum

$$S_N(\vec{Q}) = \sum_n e^{i\vec{Q}\cdot\vec{R}_n}$$

$$= \sum_{n=0}^{N-1} e^{iQna}$$

$$|S_N(Q)| = \frac{\sin(NQa/2)}{\sin(Qa/2)}$$

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)}$$

First evaluate this sum in 1D. $\vec{R}_n = na$, thus for N unit cells

Which has been evaluated previously as and leads to the Laue condition for diffraction. Looking at the regime where the Laue condition is not exactly fulfilled

$$Q = (h+\xi)a^*$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^* a/2)}{\sin([h+\xi]a^* a/2)}$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\sin(N\pi[h+\xi]) = \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi)$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

leading to peak height

$$|S_N(Q)| = \frac{\sin(N\pi\xi)}{\sin(\pi\xi)}$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

leading to peak height

$$|S_N(Q)| = \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} \approx \frac{N\pi\xi}{\pi\xi}$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^*a/2)}{\sin([h+\xi]a^*a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

leading to peak height

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

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^* a/2)}{\sin([h+\xi]a^* a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

leading to peak height

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

with half-width

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^* a/2)}{\sin([h+\xi]a^* a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

leading to peak height

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

with half-width

$$|S_N(\xi)| \to 0$$

Lattice sum in 1D

$$|S_N(Q)| = \frac{\sin(N[h+\xi]a^* a/2)}{\sin([h+\xi]a^* a/2)} = \frac{\sin(N[h+\xi]\pi)}{\sin([h+\xi]\pi)}$$

but

$$\begin{aligned}\sin(N\pi[h+\xi]) &= \sin(N\pi h)\cos(N\pi\xi) + \cos(N\pi h)\sin(N\pi\xi) \\ &= \pm\sin(N\pi\xi)\end{aligned}$$

leading to peak height

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

with half-width

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

Lattice sum in 1D

the peak area can be obtained by integration

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N \Big[\xi \Big|_{-1/2N}^{+1/2N}$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N \Big[\xi \Big|_{-1/2N}^{+1/2N} = 1$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N \Big[\xi \Big|_{-1/2N}^{+1/2N} = 1$$

consequently, the lattice sum can be written

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)| \, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N \left[\xi \right|_{-1/2N}^{+1/2N} = 1$$

consequently, the lattice sum can be written

$$|S_N(\xi)| \rightarrow \delta(\xi)$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N\Big[\xi\Big|_{-1/2N}^{+1/2N} = 1$$

consequently, the lattice sum can be written

$$|S_N(\xi)| \to \delta(\xi) \qquad\qquad \xi = \frac{Q - ha^*}{a^*} = \frac{Q - G_h}{a^*}$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N\Big[\xi\Big|_{-1/2N}^{+1/2N} = 1$$

consequently, the lattice sum can be written

$$|S_N(\xi)| \to \delta(\xi) \qquad\qquad \xi = \frac{Q - ha^*}{a^*} = \frac{Q - G_h}{a^*}$$

$$|S_N(Q)| \to a^* \sum_{G_h} \delta(Q - G_h)$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N \Big[\xi \Big|_{-1/2N}^{+1/2N} = 1$$

consequently, the lattice sum can be written

$$|S_N(\xi)| \rightarrow \delta(\xi) \qquad \xi = \frac{Q - ha^*}{a^*} = \frac{Q - G_h}{a^*}$$

$$|S_N(Q)| \rightarrow a^* \sum_{G_h} \delta(Q - G_h) = \sum_{n=0}^{N-1} e^{iQna}$$

Lattice sum in 1D

the peak area can be obtained by integration

$$\int_{-1/2N}^{+1/2N} |S_N(\xi)|\, d\xi = \int_{-1/2N}^{+1/2N} \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} d\xi \approx \int_{-1/2N}^{+1/2N} \frac{N\pi\xi}{\pi\xi} d\xi$$

$$= N \int_{-1/2N}^{+1/2N} d\xi = N\left[\xi\right|_{-1/2N}^{+1/2N} = 1$$

consequently, the lattice sum can be written

$$|S_N(\xi)| \rightarrow \delta(\xi) \qquad \xi = \frac{Q - ha^*}{a^*} = \frac{Q - G_h}{a^*}$$

$$|S_N(Q)| \rightarrow a^* \sum_{G_h} \delta(Q - G_h) = \sum_{n=0}^{N-1} e^{iQna}$$

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

Lattice sum modulus

the 1D modulus squared

Lattice sum modulus

the 1D modulus squared

$$|S_N(Q)|^2 \rightarrow Na^* \sum_{G_h} \delta(Q - G_h)$$

Lattice sum modulus

the 1D modulus squared

$$|S_N(Q)|^2 \rightarrow Na^* \sum_{G_h} \delta(Q - G_h)$$

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

Lattice sum modulus

the 1D modulus squared

$$\left|S_N(Q)\right|^2 \rightarrow Na^* \sum_{G_h} \delta(Q - G_h)$$

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

$$\left|S_N(\vec{Q})\right|^2 \rightarrow (N_1 a_1^*)(N_2 a_2^*) \sum_{\vec{G}} \delta(\vec{Q} - \vec{G}_h)$$

Lattice sum modulus

the 1D modulus squared

$$\left|S_N(Q)\right|^2 \rightarrow Na^* \sum_{G_h} \delta(Q - G_h)$$

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

$$\left|S_N(\vec{Q})\right|^2 \rightarrow (N_1 a_1^*)(N_2 a_2^*) \sum_{\vec{G}} \delta(\vec{Q} - \vec{G}_h)$$

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

Lattice sum modulus

the 1D modulus squared

$$\left|S_N(Q)\right|^2 \to Na^* \sum_{G_h} \delta(Q - G_h)$$

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

$$\left|S_N(\vec{Q})\right|^2 \to (N_1 a_1^*)(N_2 a_2^*) \sum_{\vec{G}} \delta(\vec{Q} - \vec{G}_h)$$

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

and similarly in 3D

Lattice sum modulus

the 1D modulus squared

$$\left|S_N(Q)\right|^2 \to Na^* \sum_{G_h} \delta(Q - G_h)$$

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

$$\left|S_N(\vec{Q})\right|^2 \to (N_1 a_1^*)(N_2 a_2^*) \sum_{\vec{G}} \delta(\vec{Q} - \vec{G}_h)$$

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

and similarly in 3D

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

Fourier transform of lattice function

Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

Fourier transform of lattice function

Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

$$\int_{-\infty}^{\infty} \mathcal{L}(x) e^{iQx} dx = \int_{-\infty}^{\infty} \sum_n \delta(x - na) e^{iQx} dx$$

Fourier transform of lattice function

Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

$$\int_{-\infty}^{\infty} \mathcal{L}(x) e^{iQx} dx = \int_{-\infty}^{\infty} \sum_n \delta(x - na) e^{iQx} dx = \sum_n \int_{-\infty}^{\infty} \delta(x - na) e^{iQx} dx$$

Fourier transform of lattice function

Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

$$\int_{-\infty}^{\infty} \mathcal{L}(x) e^{iQx} dx = \int_{-\infty}^{\infty} \sum_n \delta(x - na) e^{iQx} dx = \sum_n \int_{-\infty}^{\infty} \delta(x - na) e^{iQx} dx$$

$$= \sum_n e^{iQna}$$

Fourier transform of lattice function

Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

$$\int_{-\infty}^{\infty} \mathcal{L}(x) e^{iQx} dx = \int_{-\infty}^{\infty} \sum_n \delta(x - na) e^{iQx} dx = \sum_n \int_{-\infty}^{\infty} \delta(x - na) e^{iQx} dx$$
$$= \sum_n e^{iQna} = a^* \sum_h \delta(Q - ha^*)$$

Fourier transform of lattice function

Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

$$\int_{-\infty}^{\infty} \mathcal{L}(x) e^{iQx} dx = \int_{-\infty}^{\infty} \sum_n \delta(x - na) e^{iQx} dx = \sum_n \int_{-\infty}^{\infty} \delta(x - na) e^{iQx} dx$$

$$= \sum_n e^{iQna} = a^* \sum_h \delta(Q - ha^*) = a^* \sum_h \delta(Q - G_h)$$

Fourier transform of lattice function

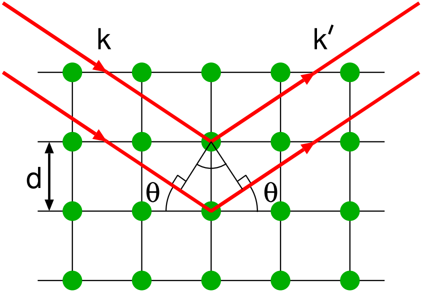
Consider the Fourier transform of the lattice function, $\mathcal{L}(x)$, (in 1-D for simplicity)

$$\int_{-\infty}^{\infty} \mathcal{L}(x) e^{iQx} dx = \int_{-\infty}^{\infty} \sum_n \delta(x - na) e^{iQx} dx = \sum_n \int_{-\infty}^{\infty} \delta(x - na) e^{iQx} dx$$
$$= \sum_n e^{iQna} = a^* \sum_h \delta(Q - ha^*) = a^* \sum_h \delta(Q - G_h)$$

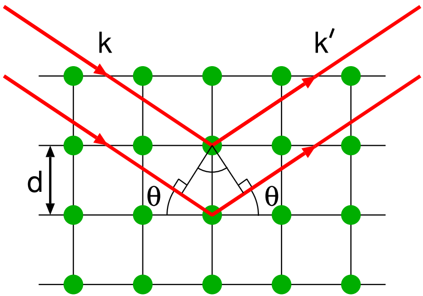
in general

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

Bragg condition

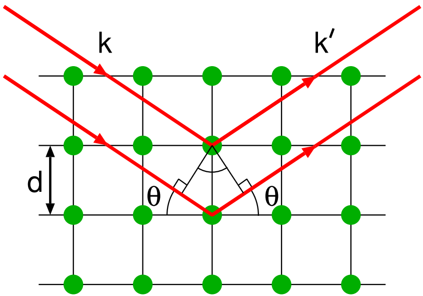


Bragg condition



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

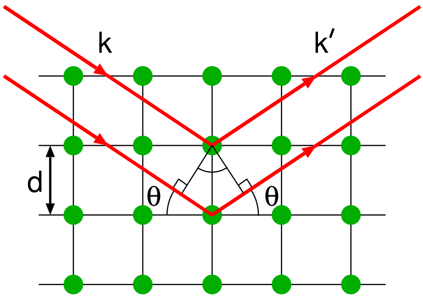
Bragg condition



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

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

Bragg condition

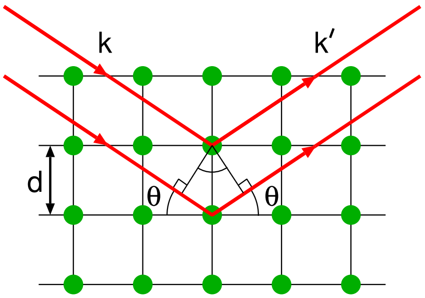


The Bragg condition for diffraction is derived by assuming specular reflection from parallel planes separated by a distance d.

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

If there is to be constructive interference, this additional distance must corresponde to an integern number of wavelengths and we get the Bragg condition

Bragg condition



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

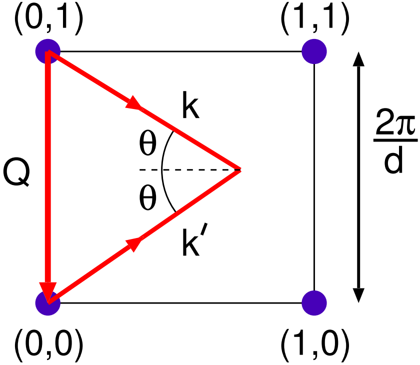
The Bragg condition for diffraction is derived by assuming specular reflection from parallel planes separated by a distance d.

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

If there is to be constructive interference, this additional distance must corresponde to an integern number of wavelengths and we get the Bragg condition

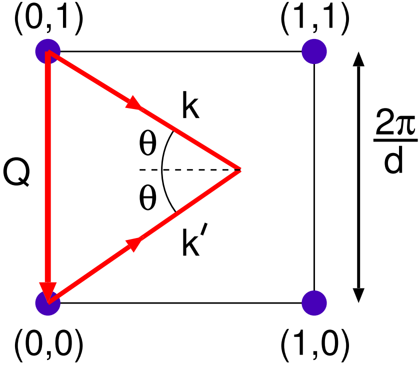
Laue condition

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



Laue condition

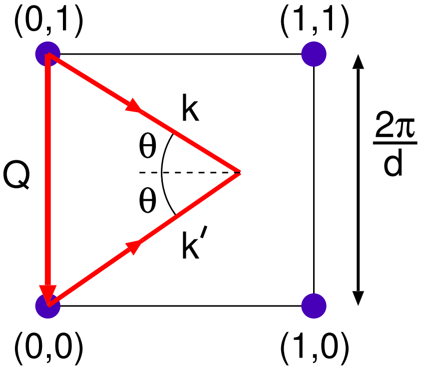
The Laue condition states that the scattering vector must be equal to a reciprocal lattice vector



Laue condition

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

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

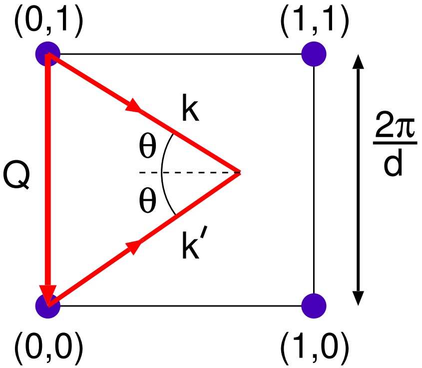


Laue condition

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

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

$$Q = 2k \sin\theta$$

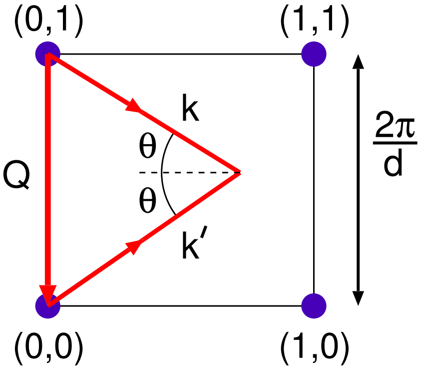


Laue condition

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

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

$$Q = 2k \sin\theta = \frac{2\pi}{d}$$



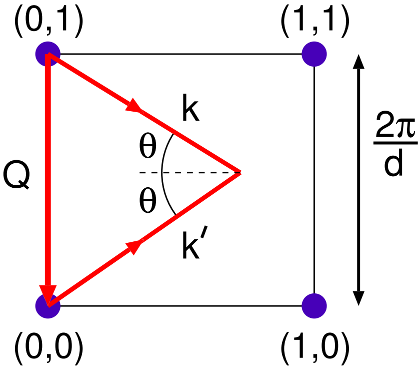
Laue condition

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

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

$$Q = 2k \sin\theta = \frac{2\pi}{d}$$

$$2d \sin\theta = \frac{2\pi}{k}$$



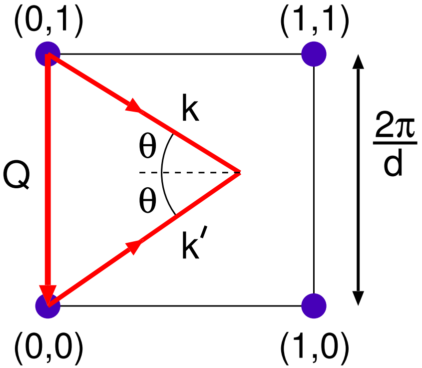
Laue condition

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

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

$$Q = 2k \sin\theta = \frac{2\pi}{d}$$

$$2d \sin\theta = \frac{2\pi}{k} = \lambda$$



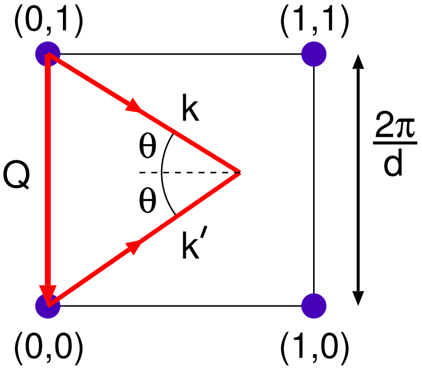
Laue condition

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

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

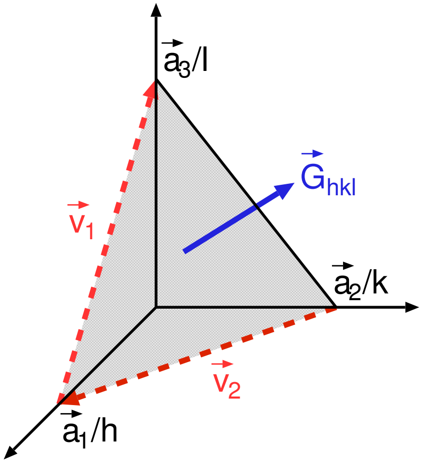
$$Q = 2k \sin\theta = \frac{2\pi}{d}$$

$$2d \sin\theta = \frac{2\pi}{k} = \lambda$$

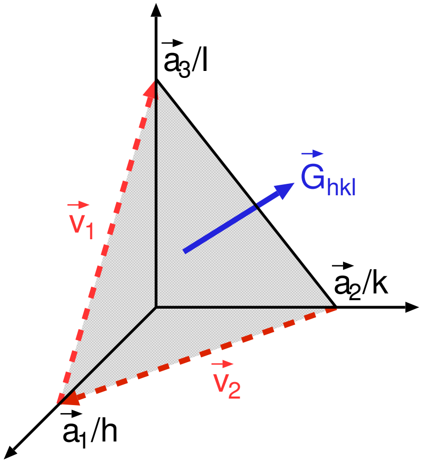


Thus the Bragg and Laue conditions are equivalent

General proof of Bragg-Laue equivalence

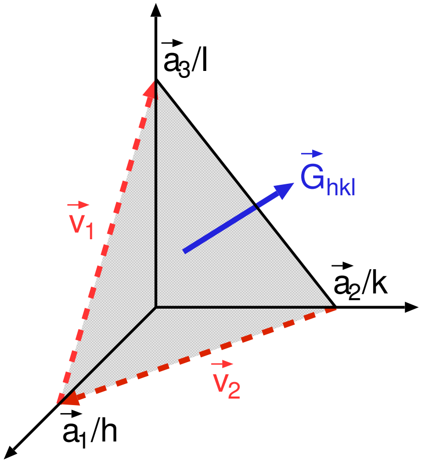


General proof of Bragg-Laue equivalence



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

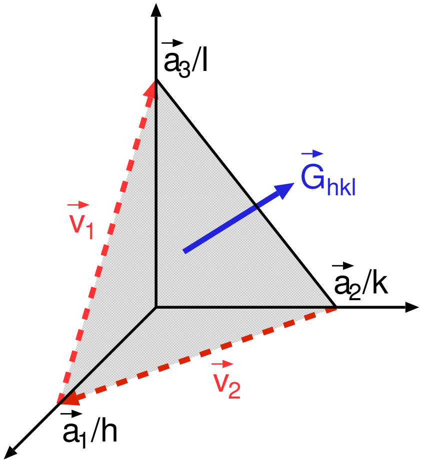
General proof of Bragg-Laue equivalence



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

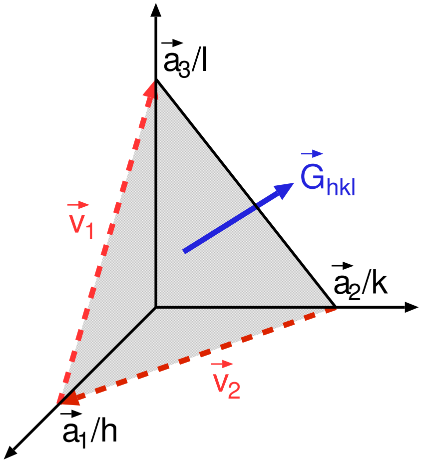
$\vec{G}_{hkl}$ is perpendicular to the planes with Miller indices (hkl)

General proof of Bragg-Laue equivalence



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) and

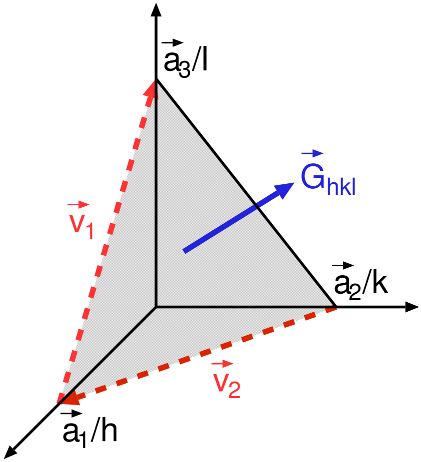


Must show that for each point in reciprocal space, there exists a set of planes in the real space lattice such that:

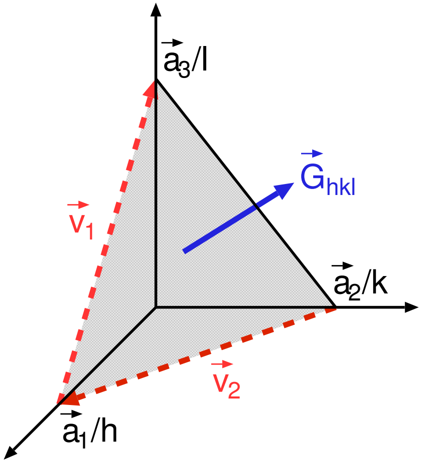
$\vec{G}_{hkl}$ is perpendicular to the planes with Miller indices (hkl) and

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

General proof of Bragg-Laue equivalence

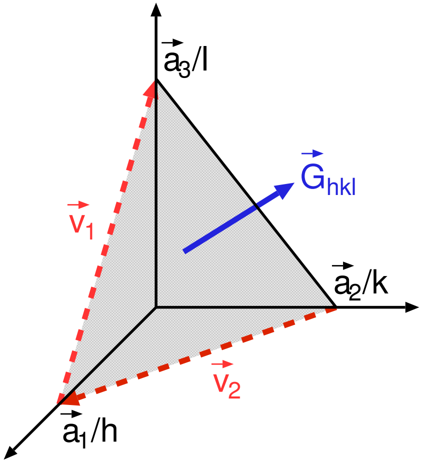


General proof of Bragg-Laue equivalence



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

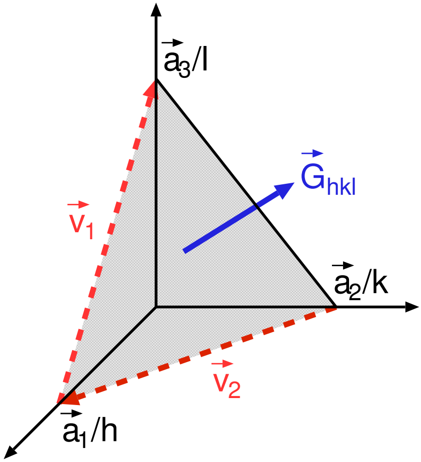
General proof of Bragg-Laue equivalence



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 $\vec{v}_2$

General proof of Bragg-Laue equivalence

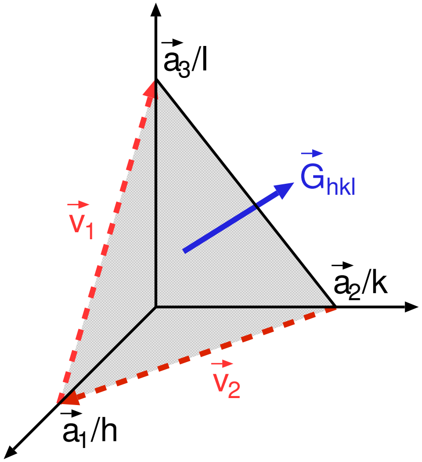


The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

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

$$\vec{v}_1 = \frac{\vec{a}_3}{l} - \frac{\vec{a}_1}{h}$$

General proof of Bragg-Laue equivalence

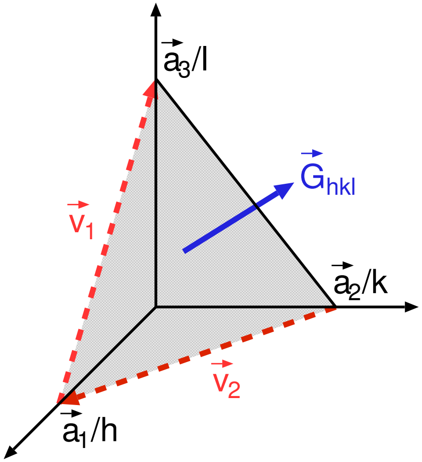


The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

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

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

General proof of Bragg-Laue equivalence



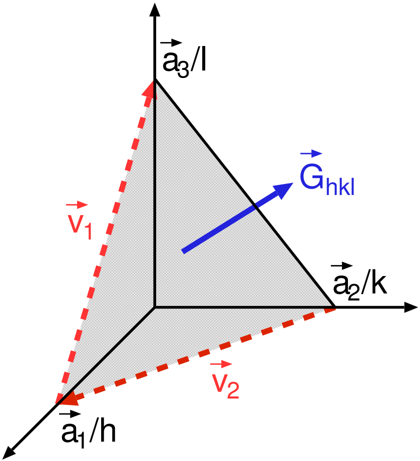
The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

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

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

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

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

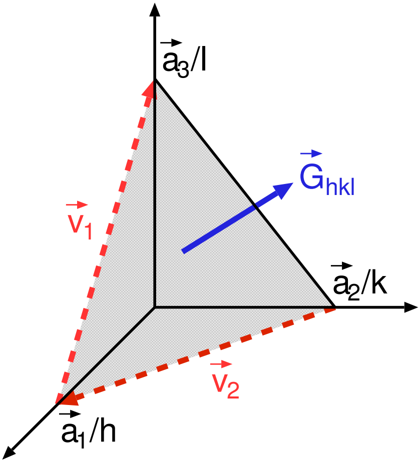
Any vector, $\vec{v}$, in this plane can be expressed as a linear combination of two non-parallel vectors, $\vec{v}_1$ and $\vec{v}_2$

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

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

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

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 $\vec{v}_2$

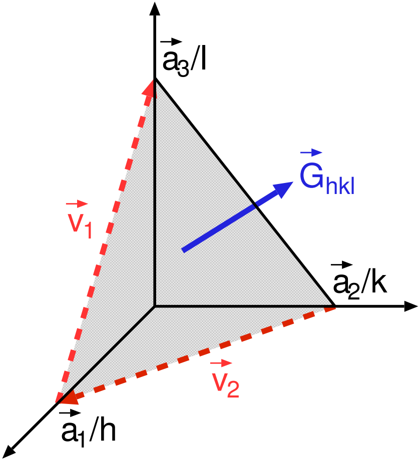
$$\vec{v}_1 = \frac{\vec{a}_3}{l} - \frac{\vec{a}_1}{h}, \quad \vec{v}_2 = \frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}$$

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

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

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

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 $\vec{v}_2$

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

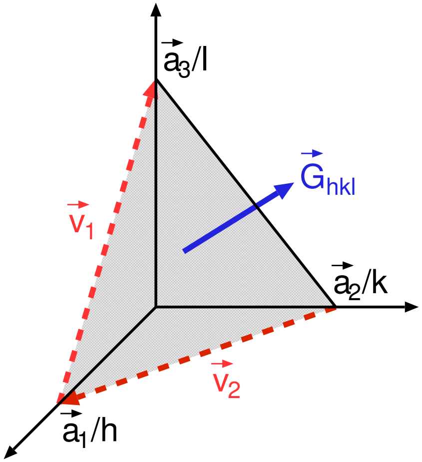
$$\vec{v} = \epsilon_1 \vec{v}_1 + \epsilon_2 \vec{v}_2$$

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

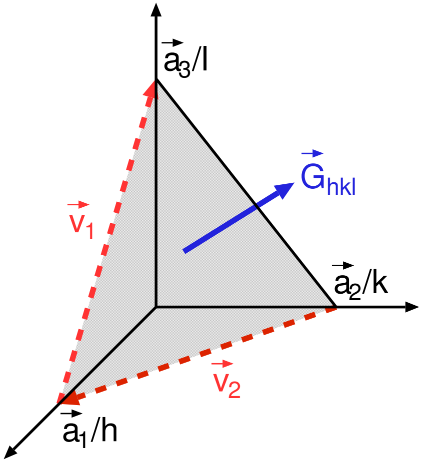
$$= 2\pi(\epsilon_2 - \epsilon_1 - \epsilon_2 + \epsilon_1) = 0$$

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

General proof of Bragg-Laue equivalence

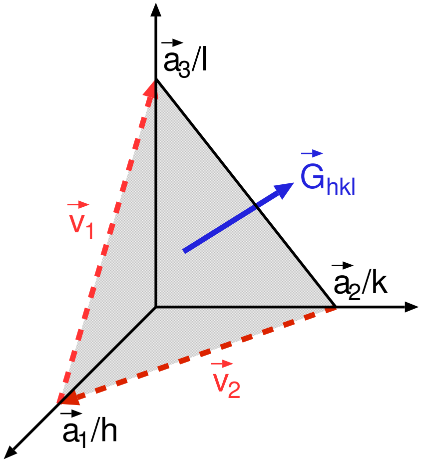


General proof of Bragg-Laue equivalence



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

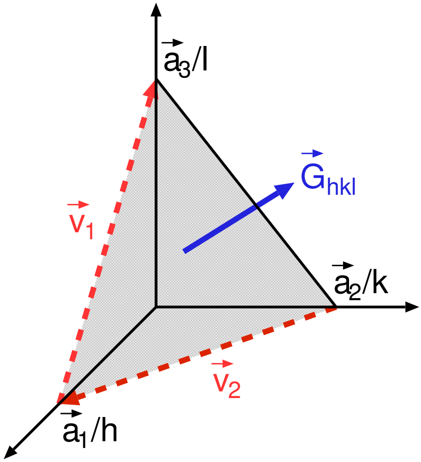
General proof of Bragg-Laue equivalence



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

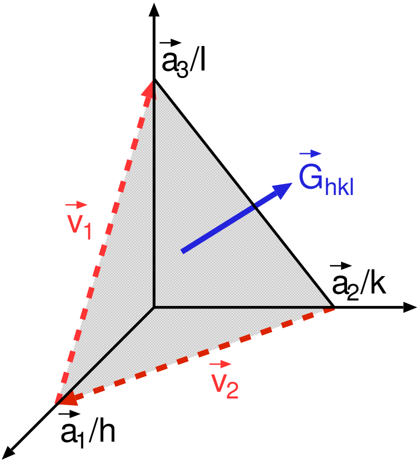


The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

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, $\vec{a}_1/h$

$$\hat{G}_{hkl} = \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|}$$

General proof of Bragg-Laue equivalence



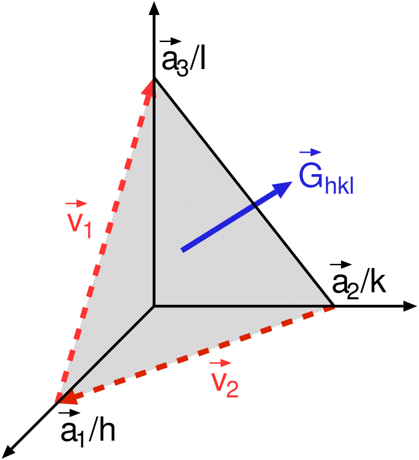
The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

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, $\vec{a}_1/h$

$$\hat{G}_{hkl} = \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|}$$

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

General proof of Bragg-Laue equivalence



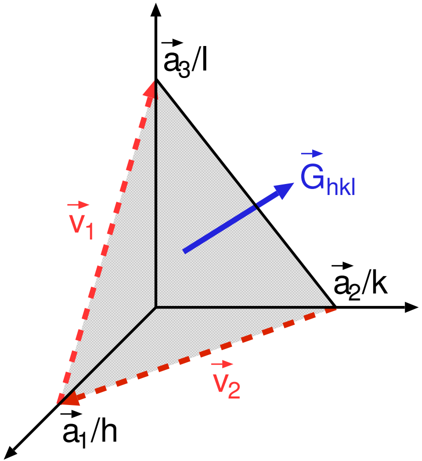
The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

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, $\vec{a}_1/h$

$$\hat{G}_{hkl} = \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|}$$

$$\hat{G}_{hkl} \cdot \frac{\vec{a}_1}{h} = \frac{(h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*)}{|\vec{G}_{hkl}|} \cdot \frac{\vec{a}_1}{h} = \frac{2\pi}{|\vec{G}_{hkl}|}$$

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

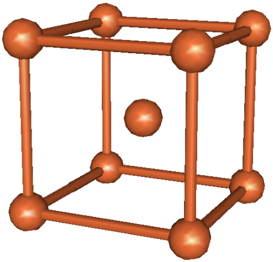
This can be computed as the projection of any vector which connects the origin to the plane onto the unit vector in the $\vec{G}_{hkl}$ direction. In this case, we choose, $\vec{a}_1/h$

$$\hat{G}_{hkl} = \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|}$$

$$\hat{G}_{hkl} \cdot \frac{\vec{a}_1}{h} = \frac{(h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*)}{|\vec{G}_{hkl}|} \cdot \frac{\vec{a}_1}{h} = \frac{2\pi}{|\vec{G}_{hkl}|} = d_{hkl}$$

BCC structure factor

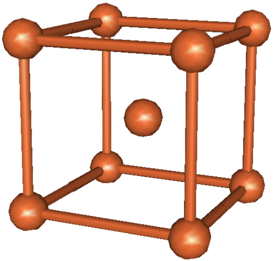
In the body centered cubic structure, there are 2 atoms in the conventional, cubic unit cell. These are located at



BCC structure factor

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

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

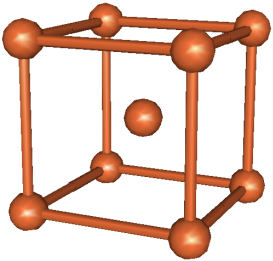


BCC structure factor

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

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

the unit cell structure factor is thus



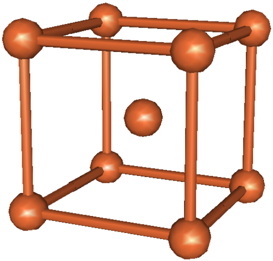
BCC structure factor

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

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

the unit cell structure factor is thus

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



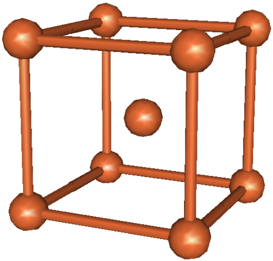
BCC structure factor

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

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

the unit cell structure factor is thus

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



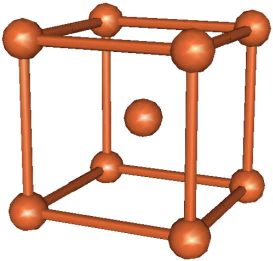
BCC structure factor

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

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

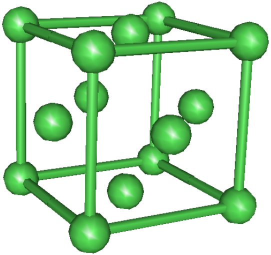
the unit cell structure factor is thus

$$\begin{aligned} F_{hkl}^{bcc} &= f(\vec{G}) \sum_j e^{i\vec{G}\cdot\vec{r}_j} \\ &= f(\vec{G}) \left(1 + e^{i\pi(h+k+l)}\right) \\ &= f(\vec{G}) \times \begin{cases} 2 & h+k+l = 2n \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$



FCC structure factor

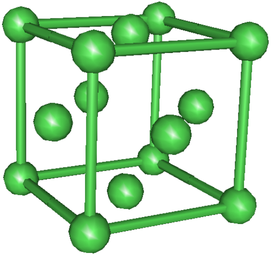
In the face centered cubic structure, there are 4 atoms in the conventional, cubic unit cell. These are located at



FCC structure factor

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

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3), \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

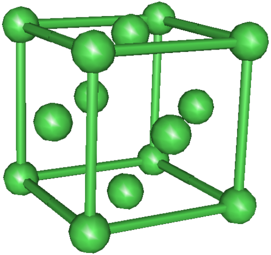


FCC structure factor

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

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3), \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

the unit cell structure factor is thus



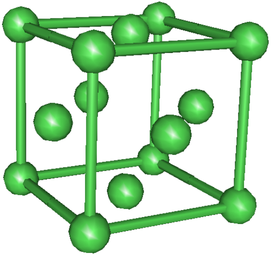
FCC structure factor

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

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3), \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

the unit cell structure factor is thus

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



FCC structure factor

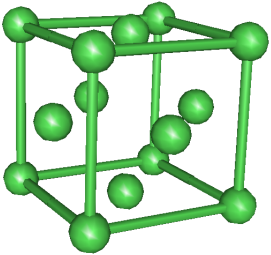
In the face centered cubic structure, there are 4 atoms in the conventional, cubic unit cell. These are located at

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3), \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

the unit cell structure factor is thus

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

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



FCC structure factor

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

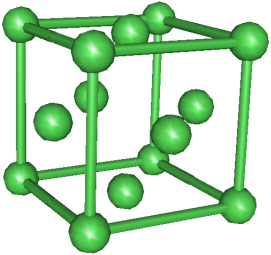
$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3), \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

the unit cell structure factor is thus

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

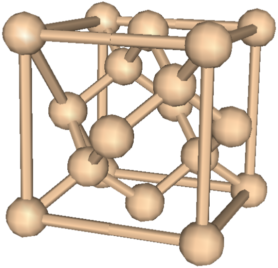
$$= f(\vec{G}) \left(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)}\right)$$

$$= f(\vec{G}) \times \begin{cases} 4 & h+k, k+l, h+l = 2n \\ 0 & \text{otherwise} \end{cases}$$



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



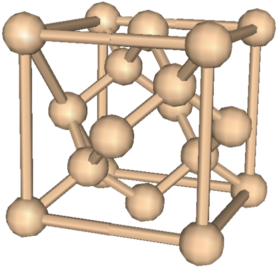
Diamond structure

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

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3) \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

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

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



Diamond structure

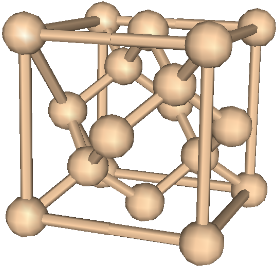
This is a face centered cubic structure with two atoms in the basis which leads to 8 atoms in the conventional unit cell. These are located at

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3) \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

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

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

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



Diamond structure

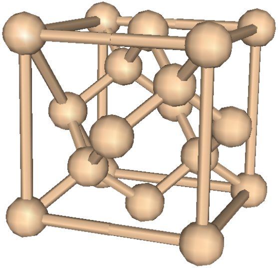
This is a face centered cubic structure with two atoms in the basis which leads to 8 atoms in the conventional unit cell. These are located at

$$\vec{r}_1 = 0, \quad \vec{r}_2 = \frac{1}{2}(\vec{a}_1 + \vec{a}_2), \quad \vec{r}_3 = \frac{1}{2}(\vec{a}_2 + \vec{a}_3) \quad \vec{r}_4 = \frac{1}{2}(\vec{a}_1 + \vec{a}_3)$$

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

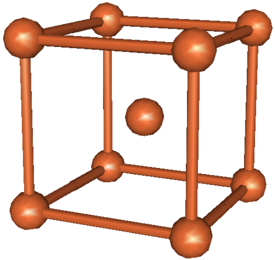
$$\vec{r}_7 = \frac{1}{4}(\vec{a}_1 + 3\vec{a}_2 + 3\vec{a}_3), \quad \vec{r}_8 = \frac{1}{4}(3\vec{a}_1 + \vec{a}_2 + 3\vec{a}_3)$$

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



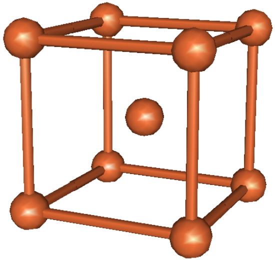
This is non-zero when h,k,l all even and $h + k + l = 4n$ or h,k,l all odd

Heteroatomic structures



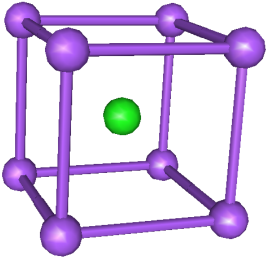
← bcc

Heteroatomic structures

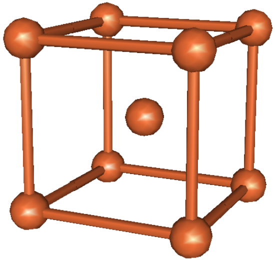


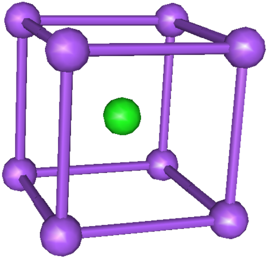
$\leftarrow$ bcc

sc $\rightarrow$



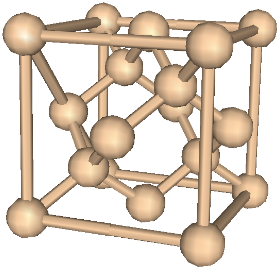
Heteroatomic structures





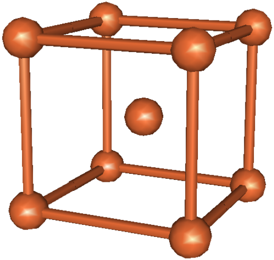
← bcc

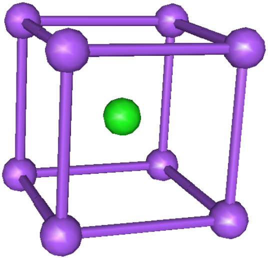
sc →



← diamond

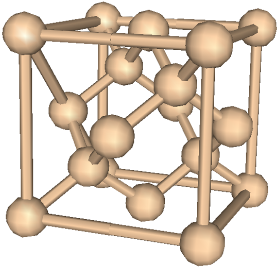
Heteroatomic structures

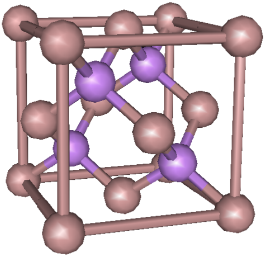




$\leftarrow$ bcc

sc $\rightarrow$





$\leftarrow$ diamond

fcc $\rightarrow$

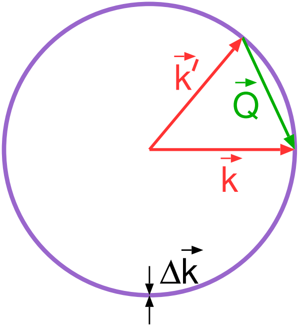
The Ewald sphere

The Ewald sphere is a construct which permits the enumeration of reflections which fulfill the Laue diffraction condition.

The Ewald sphere

The Ewald sphere is a construct which permits the enumeration of reflections which fulfill the Laue diffraction condition.

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

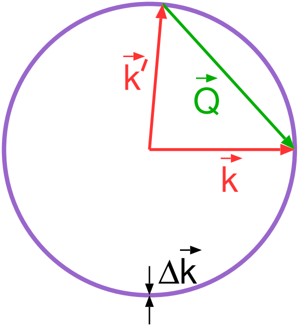


The Ewald sphere

The Ewald sphere is a construct which permits the enumeration of reflections which fulfill the Laue diffraction condition.

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

As the detector moves, $\vec{k}'$ rotates but the Ewald sphere remains constant.

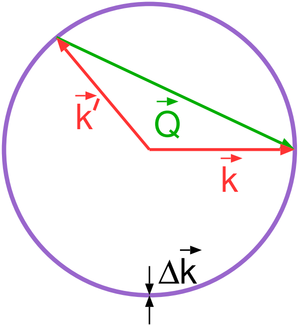


The Ewald sphere

The Ewald sphere is a construct which permits the enumeration of reflections which fulfill the Laue diffraction condition.

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

As the detector moves, $\vec{k}'$ rotates but the Ewald sphere remains constant.

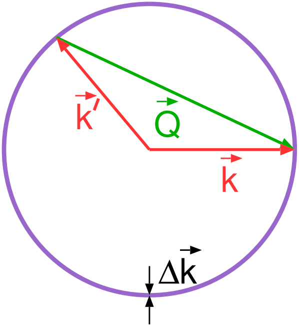


The Ewald sphere

The Ewald sphere is a construct which permits the enumeration of reflections which fulfill the Laue diffraction condition.

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

As the detector moves, $\vec{k}'$ rotates but the Ewald sphere remains constant.



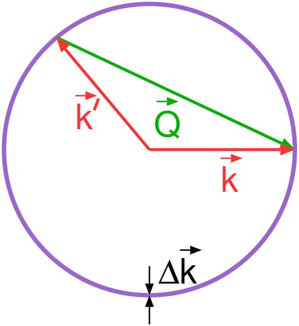
The xrayview program can be used to gain a more intuitive understanding of the Ewald sphere.

The Ewald sphere

The Ewald sphere is a construct which permits the enumeration of reflections which fulfill the Laue diffraction condition.

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

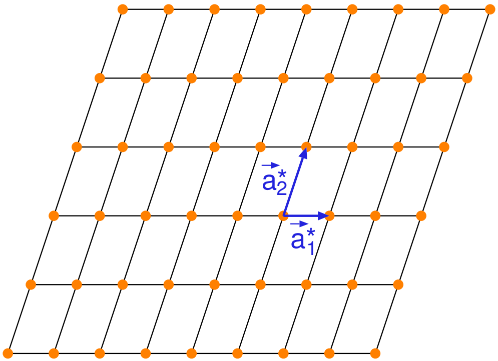
As the detector moves, $\vec{k}'$ rotates but the Ewald sphere remains constant.



The xrayview program can be used to gain a more intuitive understanding of the Ewald sphere.

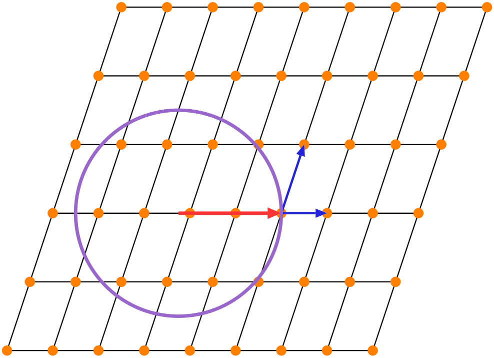
http://www.bioc.rice.edu/ georgep/xrayviewform.html

Ewald sphere & the reciprocal lattice



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

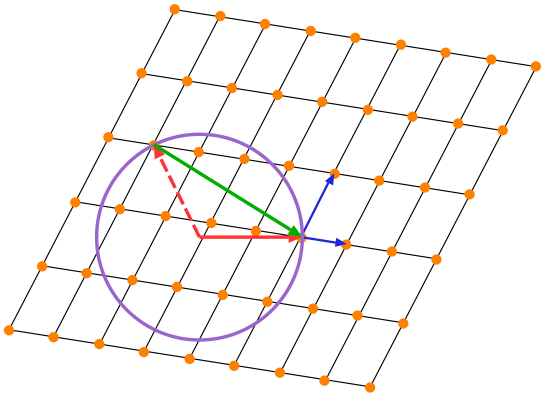
Ewald sphere & the reciprocal lattice



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 $\vec{k}$

Ewald sphere & the reciprocal lattice

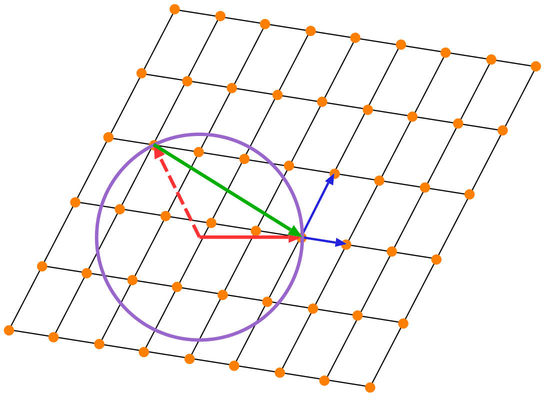


The reciprocal lattice is defined by the unit vectors $\vec{a}_1^*$ and $\vec{a}_2^*$.

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

Ewald sphere & the reciprocal lattice



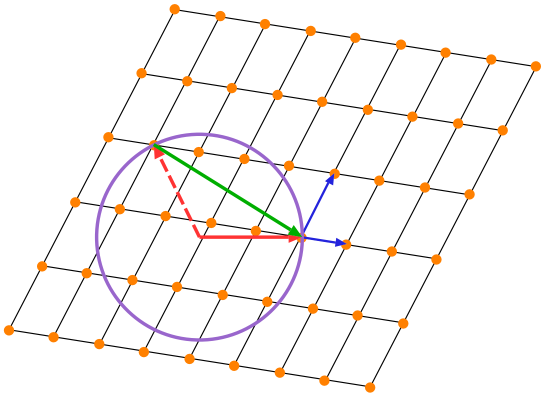
The reciprocal lattice is defined by the unit vectors $\vec{a}_1^*$ and $\vec{a}_2^*$.

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.

Ewald sphere & the reciprocal lattice



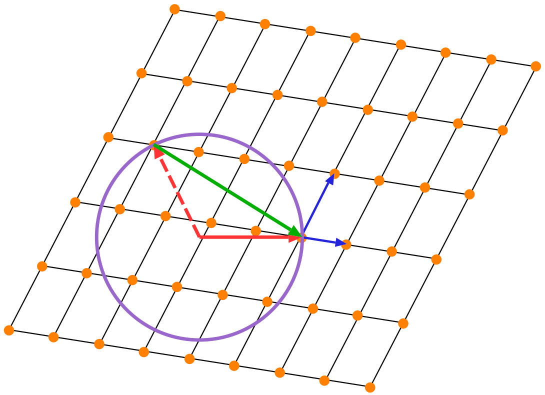
The reciprocal lattice is defined by the unit vectors $\vec{a}_1^*$ and $\vec{a}_2^*$.

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

Ewald sphere & the reciprocal lattice



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

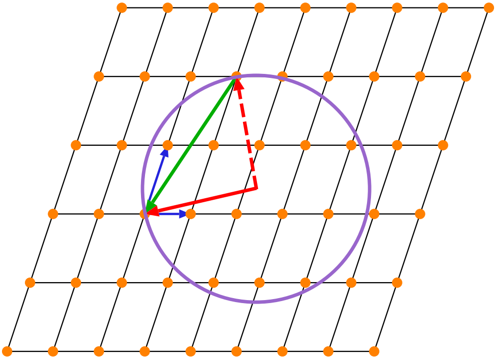
The key parameter is the relative orientation of the incident wave vector $\vec{k}$

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

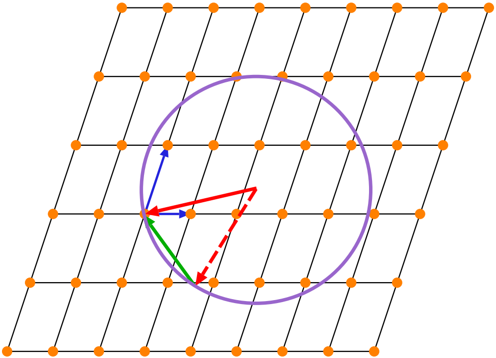
$$\vec{G}_{hlk} = h\vec{a}_1^* + k\vec{a}_2^*$$

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.

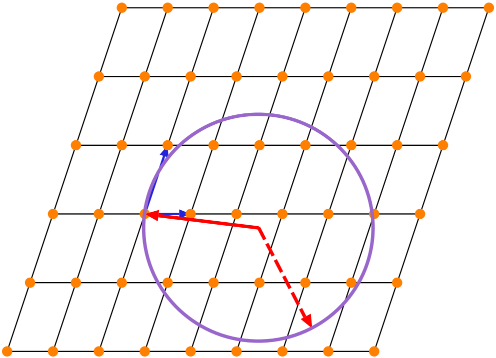
Ewald construction



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

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

Ewald construction



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

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

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