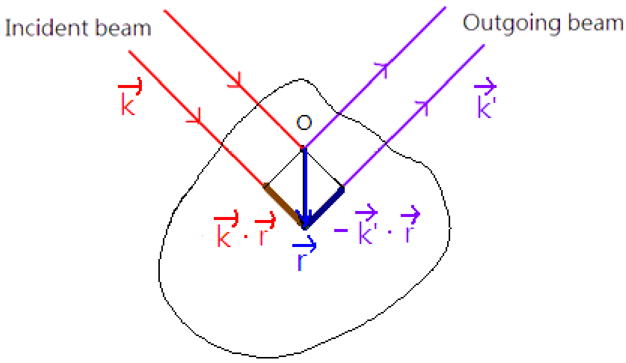
VIII kinematical theory of diffraction

8-1. total scattering amplitude



The path difference between beams scattered from the volume element $\vec{r}$ apart is

$$\left(\hat{k}\cdot\vec{r}-\widehat{k'}\cdot\vec{r}\right)\frac{2\pi}{\lambda}=\left(\vec{k}-\overrightarrow{k'}\right)\cdot\vec{r}$$

The amplitude of the wave scattered from a volume element is proportional to the local electron concentration $n(\vec{r})$.

Total scattering amplitude F

$$F=\int n(\vec{r})e^{i\left(\vec{k}-\overrightarrow{k'}\right)\cdot\vec{r}}d\vec{r}=\int n(\vec{r})e^{i\left(\vec{k}-\overrightarrow{k'}\right)\cdot\vec{r}}dV$$

Define $\Delta\vec{k}=\overrightarrow{k'}-\vec{k}$

Then

$$F=\int n(\vec{r})e^{-i\Delta\vec{k}\cdot\vec{r}}dV=\int\left(\sum_{\vec{G}}n_{\vec{G}}e^{2\pi i\vec{G}\cdot\vec{r}}\right)e^{-i\Delta\vec{k}\cdot\vec{r}}dV$$

$$F=\sum_{\vec{G}}\int n_{\vec{G}}e^{-i(\Delta\vec{k}-2\pi\vec{G})\cdot\vec{r}}dV$$

(i) When $\Delta\vec{k}=2\pi\vec{G}$,

$$F=\int n_{\vec{G}=\frac{\Delta\vec{k}}{2\pi}}dV=Vn_{\vec{G}=\frac{\Delta\vec{k}}{2\pi}}$$

$$I=FF^{*}=V^{2}n_{\vec{G}=\frac{\Delta\vec{k}}{2\pi}}n^{*}_{\vec{G}=\frac{\Delta\vec{k}}{2\pi}}$$

(ii) When $\Delta\vec{k}\neq2\pi\vec{G}$,

$$F=\sum_{\vec{G}}\int n_{\vec{G}}e^{-i(\Delta\vec{k}-2\pi\vec{G})\cdot\vec{r}}dV$$

For an infinite crystal

$$F = \sum_{\vec{G}} \int_{\infty} n_{\vec{G}} e^{-i(\Delta\vec{k} - 2\pi\vec{G})\cdot\vec{r}} dV = \sum_{\vec{G}} n_{\vec{G}} \int_{\infty} e^{-i(\Delta\vec{k} - 2\pi\vec{G})\cdot\vec{r}} dV$$

$$= \sum_{\vec{G}} n_{\vec{G}} \delta(\Delta\vec{k} - 2\pi\vec{G})$$

$$F = 0, if\ \Delta\vec{k} \neq 2\pi\vec{G}$$

Therefore, diffraction occurs at $\Delta\vec{k} = 2\pi\vec{G}$.

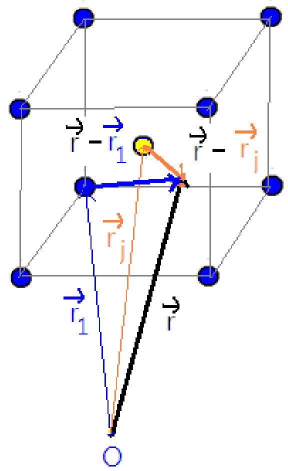
The total scattering amplitude F

$$F = \int n(\vec{r}) e^{-i\Delta\vec{k}\cdot\vec{r}} dV$$

$$= \int n(\vec{r}) e^{-2\pi i\vec{G}\cdot\vec{r}} dV = N \int_{Unit\ cell} n(\vec{r}) e^{-2\pi i\vec{G}\cdot\vec{r}} dV = NS_{\vec{G}}$$

, where $S_{\vec{G}}$ is called the structure factor.

For a unit cell, total electron concentration at $\vec{r}$ due to all atoms in the unit cell



$$n(\vec{r}) = \sum_{j=1}^{s} n_j(\vec{r} - \vec{r}_j)$$

$$S_{\vec{G}} = \int_{Unit\ cell} n(\vec{r}) e^{-2\pi i\vec{G}\cdot\vec{r}} dV = \int \sum_{j}^{s} n_j(\vec{r} - \vec{r}_j) e^{-2\pi i\vec{G}\cdot\vec{r}} dV$$

$$S_{\vec{G}} = \sum_{j}^{s} \int n_j(\vec{r} - \vec{r}_j) e^{-2\pi i\vec{G}\cdot(\vec{r} - \vec{r}_j)} e^{-2\pi i\vec{G}\cdot\vec{r}_j} dV$$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\vec{G}\cdot\vec{r}_j} f_j$$

$$f_j = \int n_j(\vec{r} - \vec{r}_j) e^{-2\pi i\vec{G}\cdot(\vec{r}-\vec{r}_j)} dV$$

, where f_j is so called form factor.

The scattering amplitude is then expressed as

$$\mathrm{F} = \mathrm{N}S_{\vec{G}} = N\sum_{j}^{s} e^{-2\pi i\vec{G}\cdot\vec{r}_j} f_j$$

8-2. form factor calculation

The meaning of form factor is equivalent to the total charge of an atom, which can be obtained by a direct calculation.

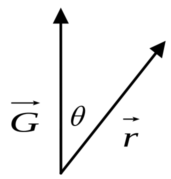
With the integral extended over the electron concentration associated with a single atom, set the origin at the atom

$$f_j = \int n_j(\vec{r} - \vec{r}_j) e^{-2\pi i\vec{G}\cdot(\vec{r}-\vec{r}_j)} dV = \int n_j(\vec{r}) e^{-2\pi i\vec{G}\cdot\vec{r}} dV$$

$$f_j = \int_{\mathrm{r}} \int_{\theta}^{\pi} \int_{\phi}^{2\pi} n_j(r) e^{-2\pi i G r\cos\theta} dr(r d\theta)(r\sin\theta d\phi)$$

$$f_j = \int_{\mathrm{r}} \int_{\theta}^{\pi} \int_{\phi}^{2\pi} n_j(r) e^{-2\pi i G r\cos\theta} r^2 \sin\theta dr d\theta d\phi$$

, where we use $\vec{G}\cdot\vec{r} = Gr\cos\theta$ and assume $n_j(\vec{r}) = n_j(r)$.



$$f_j = 2\pi \int_{\mathrm{r}} n_j(r) r^2 dr \int_{\theta=0}^{\pi} e^{-2\pi i G r\cos\theta} \sin\theta d\theta$$

$$f_j = 2\pi \int_{r} n_j(r) r^2 dr \int_{-1}^{1} e^{-2\pi i G r \cos\theta} d(\cos\theta)$$

$$f_j = 2\pi \int_{r} n_j(r) r^2 dr \frac{e^{-2\pi i G r} - e^{2\pi i G r}}{-2\pi i G r}$$

$$= 4\pi \int_{r} n_j(r) r^2 dr \frac{\sin(2\pi G r)}{2\pi G r}$$

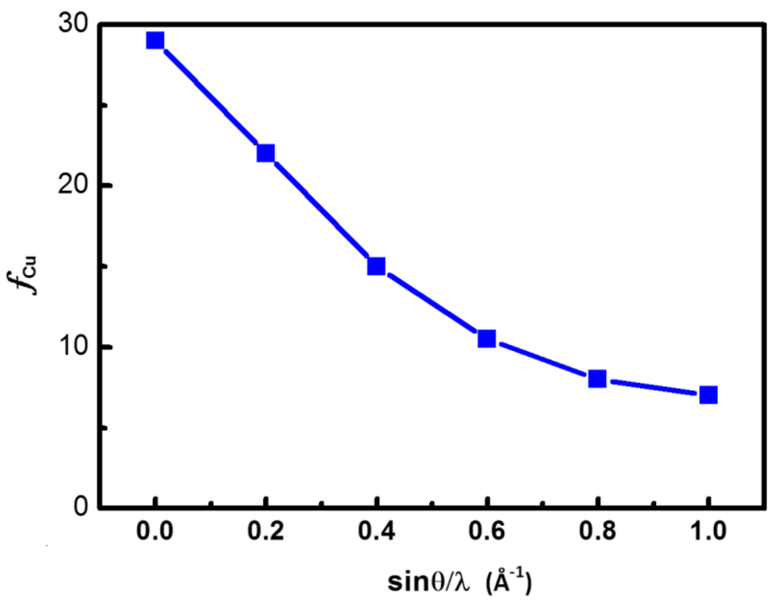
If total electron concentration were concentrated at r=0,

$$f_j = 4\pi \int_{r} n_j(r) r^2 dr = Z$$

, where Z is the total number of electron in an atom.

In fact, f_j depends on $\frac{\sin\theta}{\lambda}$.

For example, the form factor of Cu is



8-3. structure factor calculation

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i \vec{G}\cdot\vec{r}_j} f_j = \sum_{j}^{s} e^{-2\pi i (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(u_j\vec{a} + v_j\vec{b} + w_j\vec{c})} f_j$$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i (hu_j + kv_j + lw_j)} f_j$$

For example：

(a) one atom in a unit cell at [000]

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(u_j\vec{a} + v_j\vec{b} + w_j\vec{c})} f_j$$

$$S_{\vec{G}} = e^{-2\pi i (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(0\vec{a} + 0\vec{b} + 0\vec{c})} f = f$$

(b) base-centered cell : two atoms at [000] and $\left[\frac{1}{2}\frac{1}{2}0\right]$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(u_j\vec{a} + v_j\vec{b} + w_j\vec{c})} f_j$$

$$S_{\vec{G}} = f\left[e^{-2\pi i (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot(0\vec{a} + 0\vec{b} + 0\vec{c})} + e^{-2\pi i (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)\cdot\left(\frac{1}{2}\vec{a} + \frac{1}{2}\vec{b} + 0\vec{c}\right)}\right]$$

$$S_{\vec{G}} = f\left[e^{0} + e^{-2\pi i \left(\frac{h}{2} + \frac{k}{2} + 0\right)}\right] = f\left[1 + e^{-\pi i (h+k)}\right]$$

Hence,

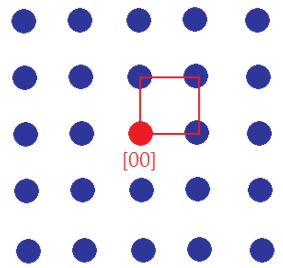
$S_{\vec{G}} = 2f$ if h and k unmixed.

$S_{\vec{G}} = 0$ if h and k mixed (one even; one odd).

The meaning of the reflection condition (reflection rule)

Suppose that we have a square lattice

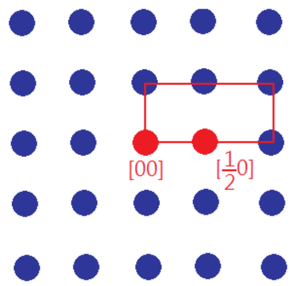
(a) Primitive unit cell：one atom at [00]



$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i(h\vec{a}^*+k\vec{b}^*)\cdot(u_j\vec{a}+v_j\vec{b})} f_j$$

$$S_{\vec{G}} = e^{-2\pi i(h\vec{a}^*+k\vec{b}^*)\cdot(0\vec{a}+0\vec{b})} f = f$$

(b) Unit cell：two atoms at [00] $[\frac{1}{2}0]$



$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i(h\vec{a}^*+k\vec{b}^*)\cdot(u_j\vec{a}+v_j\vec{b})} f_j$$

$$S_{\vec{G}} = f\left[e^{-2\pi i(h\vec{a}^*+k\vec{b}^*)\cdot(0\vec{a}+0\vec{b})} + e^{-2\pi i(h\vec{a}^*+k\vec{b}^*)\cdot\left(\frac{1}{2}\vec{a}+0\vec{b}\right)}\right]$$

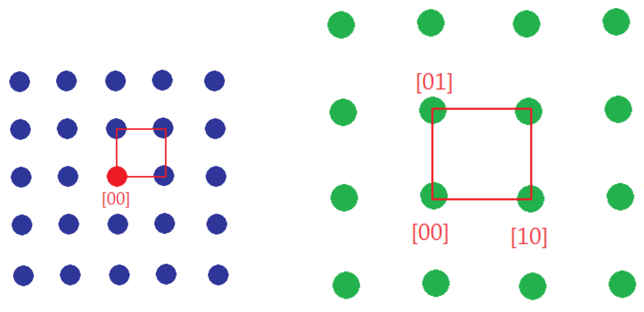
$$S_{\vec{G}} = f\left[e^{0} + e^{-2\pi i\left(\frac{h}{2}\right)}\right] = f\left[1 + e^{-\pi i(h)}\right]$$

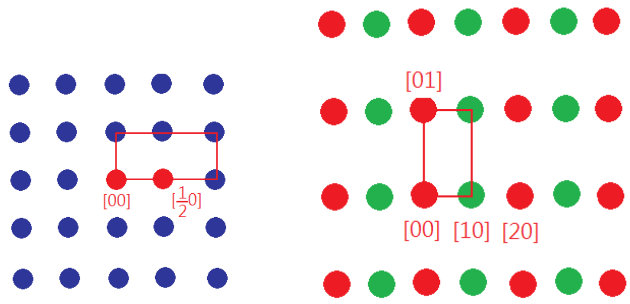
Hence,

$S_{\vec{G}} = 2f$ if h is even.
$S_{\vec{G}} = 0$ if h is odd.

The reflection conditions for the case (b) are

$S_{\vec{G}} = 2f$ if h is even.
$S_{\vec{G}} = 0$ if h is odd.





The reflection conditions remove the lattice points [odd, 0] in the reciprocal lattice.

Therefore, the meaning of the reflection rule is to remove the additional lattice points due to the selection of unit cell.

After the substraction, the reciprocal lattice structures derived from both cases (primitive unit cell and unit cell) become the same.

(c) body centered cell : two atoms at [000] and $\left[\frac{1}{2}\frac{1}{2}\frac{1}{2}\right]$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\left(h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}\right)\cdot\left(u_j\vec{a}+v_j\vec{b}+w_j\vec{c}\right)} f_j$$

$$S_{\vec{G}} = f\left[e^{-2\pi i\left(h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}\right)\cdot\left(0\vec{a}+0\vec{b}+0\vec{c}\right)} + e^{-2\pi i\left(h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}\right)\cdot\left(\frac{1}{2}\vec{a}+\frac{1}{2}\vec{b}+\frac{1}{2}\vec{c}\right)}\right]$$

$$S_{\vec{G}} = f\left[e^{0} + e^{-2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)}\right] = f\left[1 + e^{-\pi i(h+k+l)}\right]$$

Hence,

$S_{\vec{G}} = 2f$ if $h+k+l$ is even.
$S_{\vec{G}} = 0$ if $h+k+l$ is odd.

(d) face-centered cubic cell :

four atoms at [000], $\left[\frac{1}{2}\frac{1}{2}0\right]$, $\left[\frac{1}{2}0\frac{1}{2}\right]$, $\left[0\frac{1}{2}\frac{1}{2}\right]$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\left(h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}\right)\cdot\left(u_j\vec{a}+v_j\vec{b}+w_j\vec{c}\right)} f_j$$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\left(hu_j+kv_j+lw_j\right)} f_j$$

$$S_{\vec{G}} = f\left[e^{0} + e^{-2\pi i\left(\frac{h}{2}+\frac{k}{2}\right)} + e^{-2\pi i\left(\frac{h}{2}+\frac{l}{2}\right)} + e^{-2\pi i\left(\frac{k}{2}+\frac{l}{2}\right)}\right]$$
$$= f\left[1 + e^{-\pi i(h+k)} + e^{-\pi i(h+l)} + e^{-\pi i(k+l)}\right]$$

Hence,

$S_{\vec{G}} = 4f$ if h, k and l are unmixed.
$S_{\vec{G}} = 0$ if h, k and l are mixed.

(e) close-packed hexagonal cell

Two atoms are at [000] and $\left[\frac{2}{3}\frac{1}{3}\frac{1}{2}\right]$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\left(hu_j+kv_j+lw_j\right)} f_j$$

$$S_{\vec{G}} = f\left[e^{0} + e^{-2\pi i\left(\frac{2h}{3}+\frac{k}{3}+\frac{l}{2}\right)}\right] = f\left[1 + e^{-2\pi i\left(\frac{2h+k}{3}+\frac{l}{2}\right)}\right]$$

$$\left|S_{\vec{G}}\right|^2 = f^2\left[1+e^{-2\pi i\left(\frac{2h}{3}+\frac{k}{3}+\frac{l}{2}\right)}\right]\left[1+e^{2\pi i\left(\frac{2h}{3}+\frac{k}{3}+\frac{l}{2}\right)}\right]$$

$$\left|S_{\vec{G}}\right|^2 = f^2\left[1+e^{2\pi i\left(\frac{2h}{3}+\frac{k}{3}+\frac{l}{2}\right)}+e^{-2\pi i\left(\frac{2h}{3}+\frac{k}{3}+\frac{l}{2}\right)}+1\right]$$
$$= f^2\left\{2+2\cos\left[2\pi\left(\frac{2h}{3}+\frac{k}{3}+\frac{l}{2}\right)\right]\right\}$$

$$\left|S_{\vec{G}}\right|^2 = 4f^2\cos^2\left(\frac{2h+k}{3}+\frac{l}{2}\right)\pi$$

2h+k	L	$\left\|S_{\vec{G}}\right\|^2$
3m	Odd	0
3m	Even	$4f^2$
3m±1	Odd	$3f^2$
3m±1	Even	f^2

(f) ZnS has four Zinc and four sulfur atoms per unit cell

Zn: $\left[\frac{1}{4}\frac{1}{4}\frac{1}{4}\right]$+ face centering translation
S: [000] + face centering translation

$$S_{\vec{G}} = \sum_j^s e^{-2\pi i\left(h\vec{a}^*+k\vec{b}^*+l\vec{c}^*\right)\cdot\left(u_j\vec{a}+v_j\vec{b}+w_j\vec{c}\right)}f_j$$

$$S_{\vec{G}} = \sum_j^s e^{-2\pi i\left(hu_j+kv_j+lw_j\right)}f_j$$

$$S_{\vec{G}} = f_s\left[1+e^{-\pi i(h+k)}+e^{-\pi i(h+l)}+e^{-\pi i(k+l)}\right] + f_{Zn}\left[1+e^{-\pi i(h+k)}+e^{-\pi i(h+l)}+e^{-\pi i(k+l)}\right]e^{-2\pi i\left(\frac{h}{4}+\frac{k}{4}+\frac{l}{4}\right)}$$

$$S_{\vec{G}} = \left[1+e^{-\pi i(h+k)}+e^{-\pi i(h+l)}+e^{-\pi i(k+l)}\right]\left(f_s+f_{Zn}e^{-2\pi i\left(\frac{h}{4}+\frac{k}{4}+\frac{l}{4}\right)}\right)$$
$$= S_{fcc}\left(f_s+f_{Zn}e^{-\frac{\pi}{2}i(h+k+l)}\right)$$

$$\left|S_{\vec{G}}\right|^2 = \left|S_{fcc}\right|^2\left[f_s+f_{Zn}e^{-\frac{\pi}{2}i(h+k+l)}\right]\left[f_s+f_{Zn}e^{\frac{\pi}{2}i(h+k+l)}\right]$$

$$\left|S_{\vec{G}}\right|^2 = \left|S_{fcc}\right|^2\left[{f_s}^2+{f_{Zn}}^2+2f_sf_{Zn}\cos\frac{\pi}{2}(h+k+l)\right]$$

Hence,

$\left|S_{\vec{G}}\right|^2 = 16\left({f_s}^2 + {f_{Zn}}^2\right)$ if h+k+l is odd.

$\left|S_{\vec{G}}\right|^2 = 16(f_s - f_{Zn})^2$ if h+k+l is an odd multiple of 2.

$\left|S_{\vec{G}}\right|^2 = 16(f_s + f_{Zn})^2$ if h+k+l is an even multiple of 2

8-4. Shape effect

For a finite crystal; assuming rectangular volume

$$F = \sum_{\vec{G}} \int n_{\vec{G}} e^{-i(\Delta\vec{k}-2\pi\vec{G})\cdot\vec{r}} dV$$

For a particular $\vec{G}$, if $\Delta\vec{k} - 2\pi\vec{G} = \vec{D} \neq 0$

$$F = \sum_{\vec{G}} \int n_{\vec{G}} e^{-i\vec{D}\cdot\vec{r}} dV = \int n_{\vec{G}} e^{-i\vec{D}\cdot(x\vec{a}+y\vec{b}+z\vec{c})} dxdydz$$

$$F = \sum_{x=0}^{M-1} \sum_{y=0}^{N-1} \sum_{z=0}^{L-1} n_{\vec{G}} e^{-i\vec{D}\cdot(x\vec{a}+y\vec{b}+z\vec{c})}$$

$$= n_{\vec{G}} \sum_{x=0}^{M-1} e^{-i\vec{D}\cdot x\vec{a}} \sum_{y=0}^{N-1} e^{-i\vec{D}\cdot y\vec{b}} \sum_{z=0}^{L-1} e^{-i\vec{D}\cdot z\vec{c}}$$

$$F = n_{\vec{G}} \frac{1-e^{-iM\vec{D}\cdot\vec{a}}}{1-e^{-i\vec{D}\cdot\vec{a}}} \frac{1-e^{-iN\vec{D}\cdot\vec{b}}}{1-e^{-i\vec{D}\cdot\vec{b}}} \frac{1-e^{-iL\vec{D}\cdot\vec{c}}}{1-e^{-i\vec{D}\cdot\vec{c}}}$$

, where we use $\sum_{m=0}^{M-1} t^m = \frac{1-t^M}{1-t}$

$$F = n_{\vec{G}} \left[\frac{e^{-i\frac{M}{2}\vec{D}\cdot\vec{a}}}{e^{-i\frac{1}{2}\vec{D}\cdot\vec{a}}} \left(\frac{e^{i\frac{M}{2}\vec{D}\cdot\vec{a}} - e^{-i\frac{M}{2}\vec{D}\cdot\vec{a}}}{e^{i\frac{1}{2}\vec{D}\cdot\vec{a}} - e^{-i\frac{1}{2}\vec{D}\cdot\vec{a}}} \right) \right] \left[\frac{e^{-i\frac{N}{2}\vec{D}\cdot\vec{b}}}{e^{-i\frac{1}{2}\vec{D}\cdot\vec{b}}} \left(\frac{e^{i\frac{N}{2}\vec{D}\cdot\vec{b}} - e^{-i\frac{N}{2}\vec{D}\cdot\vec{b}}}{e^{i\frac{1}{2}\vec{D}\cdot\vec{b}} - e^{-i\frac{1}{2}\vec{D}\cdot\vec{b}}} \right) \right] \left[\frac{e^{-i\frac{L}{2}\vec{D}\cdot\vec{c}}}{e^{-i\frac{1}{2}\vec{D}\cdot\vec{c}}} \left(\frac{e^{i\frac{L}{2}\vec{D}\cdot\vec{c}} - e^{-i\frac{L}{2}\vec{D}\cdot\vec{c}}}{e^{i\frac{1}{2}\vec{D}\cdot\vec{c}} - e^{-i\frac{1}{2}\vec{D}\cdot\vec{c}}} \right) \right]$$

$$F = n_{\vec{G}} \left[e^{-i\frac{M-1}{2}\vec{D}\cdot\vec{a}} \left(\frac{\sin\left(\frac{M}{2}\vec{D}\cdot\vec{a}\right)}{\sin\left(\frac{1}{2}\vec{D}\cdot\vec{a}\right)} \right) \right] \left[e^{-i\frac{N-1}{2}\vec{D}\cdot\vec{a}} \left(\frac{\sin\left(\frac{N}{2}\vec{D}\cdot\vec{b}\right)}{\sin\left(\frac{1}{2}\vec{D}\cdot\vec{b}\right)} \right) \right] \left[e^{-i\frac{L-1}{2}\vec{D}\cdot\vec{c}} \left(\frac{\sin\left(\frac{L}{2}\vec{D}\cdot\vec{c}\right)}{\sin\left(\frac{1}{2}\vec{D}\cdot\vec{c}\right)} \right) \right]$$

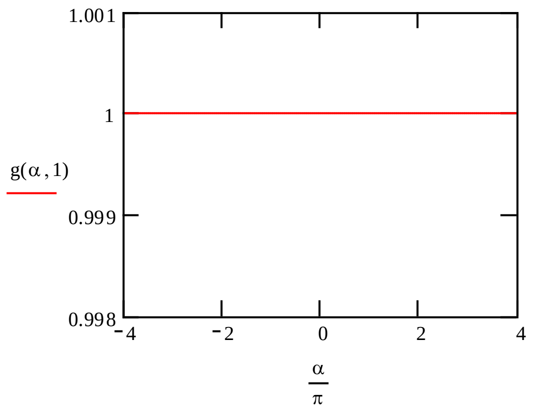
$$I = FF^* = n_{\vec{G}} n_{\vec{G}}^* \left(\frac{\sin M\alpha}{\sin\alpha}\right)^2 \left(\frac{\sin N\beta}{\sin\beta}\right)^2 \left(\frac{\sin L\gamma}{\sin\gamma}\right)^2$$

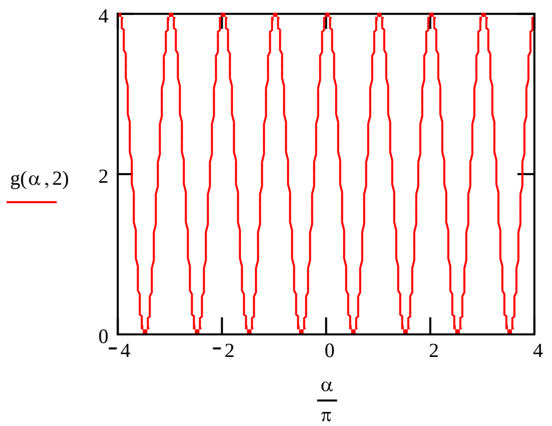
, where

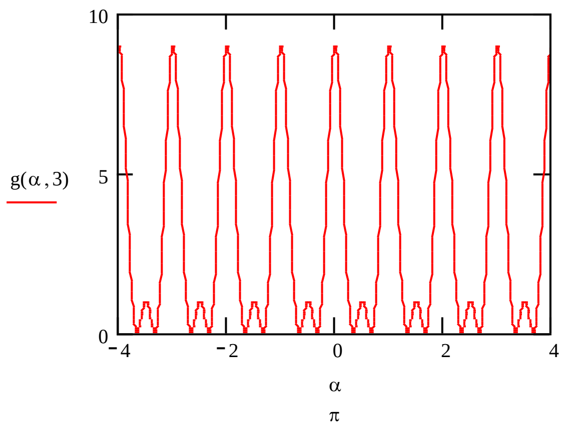
$\alpha = \frac{1}{2}\vec{D}\cdot\vec{a},\ \beta = \frac{1}{2}\vec{D}\cdot\vec{b},\ \gamma = \frac{1}{2}\vec{D}\cdot\vec{c}$, and $\vec{D} = \Delta\vec{k} - 2\pi\vec{G}$

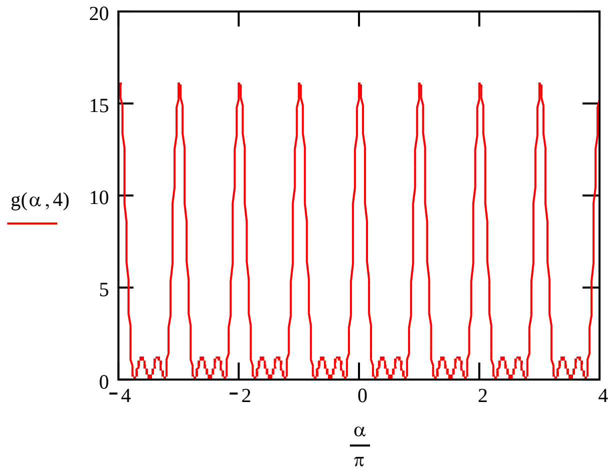
$$\alpha := -4\pi, -3.99\pi .. 4\pi$$

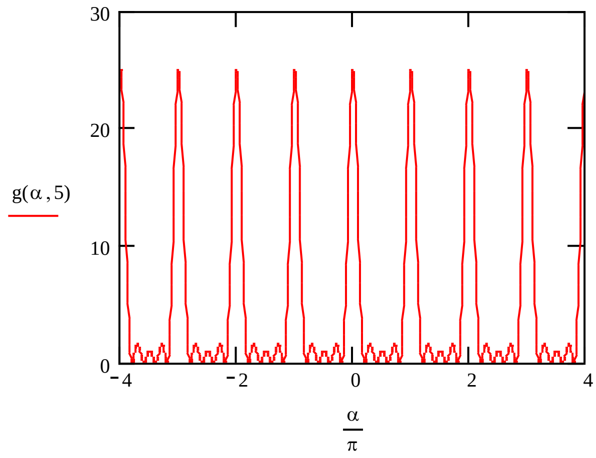
$$g(\alpha, N) := \left(\frac{\sin(N \cdot \alpha)}{\sin(\alpha)}\right)^2$$

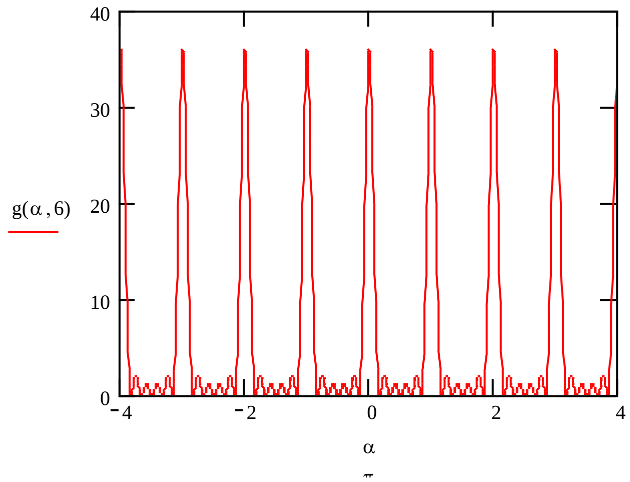


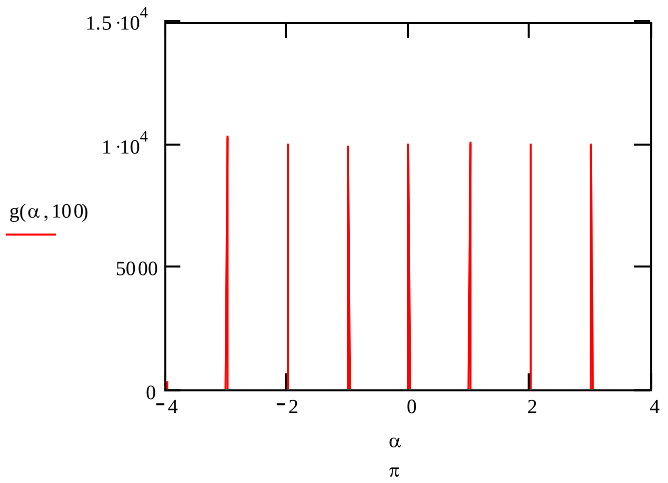





20
15
10
5
0
g(α, 4)
-4
-2
0
2
4
α
π


30
20
10
0
g(α, 5)
-4
-2
0
2
4
α
π


40
30
20
10
0
g(α, 6)
-4
-2
0
2
4
α



Considering the intensity

$$I = FF^* = n_{\vec{G}} n_{\vec{G}}^* \left(\frac{\sin M\alpha}{\sin \alpha}\right)^2 \left(\frac{\sin N\beta}{\sin \beta}\right)^2 \left(\frac{\sin L\gamma}{\sin \gamma}\right)^2$$

1st min occurs at $\sin M\alpha = 0$, $\sin N\beta = 0$, and $\sin L\gamma = 0$
i.e. $M\alpha = \pi$, $\sin N\beta = \pi$, and $\sin L\gamma = \pi$

Substituting

$$\alpha = \frac{1}{2}\vec{D}\cdot\vec{a},\ \beta = \frac{1}{2}\vec{D}\cdot\vec{b},\ \gamma = \frac{1}{2}\vec{D}\cdot\vec{c}, \text{and } \vec{D} = \Delta\vec{k} - 2\pi\vec{G}$$

We can obtain

$$\left(\Delta\vec{k} - 2\pi\vec{G}\right)\cdot\vec{a} = \frac{2\pi}{M}$$
$$\left(\Delta\vec{k} - 2\pi\vec{G}\right)\cdot\vec{b} = \frac{2\pi}{N}$$
$$\left(\Delta\vec{k} - 2\pi\vec{G}\right)\cdot\vec{c} = \frac{2\pi}{L}$$

or

$$\left(\frac{\Delta\vec{k}}{2\pi} - \vec{G}\right)\cdot\vec{a} = \frac{1}{M}$$
$$\left(\frac{\Delta\vec{k}}{2\pi} - \vec{G}\right)\cdot\vec{b} = \frac{1}{N}$$
$$\left(\frac{\Delta\vec{k}}{2\pi} - \vec{G}\right)\cdot\vec{c} = \frac{1}{L}$$

Therefore, for a finite crystal, the diffracted intensity is finite based on the condition below.

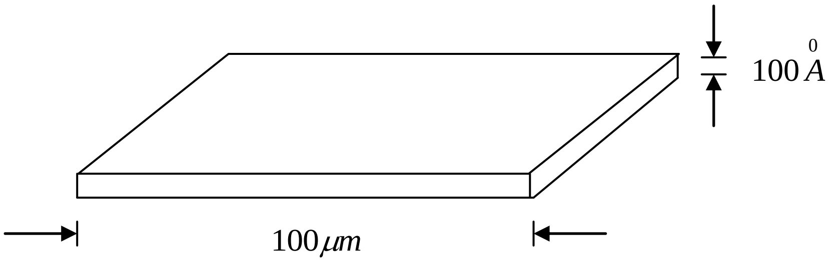
$$I \neq 0 \ if$$

$$\left|\left(\frac{\Delta\vec{k}}{2\pi} - \vec{G}\right)\cdot\vec{a}\right| < \frac{1}{M}$$

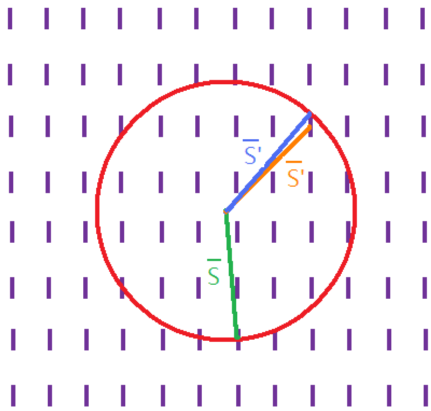
$$\left|\left(\frac{\Delta\vec{k}}{2\pi} - \vec{G}\right)\cdot\vec{b}\right| < \frac{1}{N}$$

$$\left|\left(\frac{\Delta\vec{k}}{2\pi} - \vec{G}\right)\cdot\vec{c}\right| < \frac{1}{L}$$

Example #1: for a very thin sample



Ewald sphere construction



$\bar{S} - \bar{S}' = \bar{G}$

, where $\vec{S} = \frac{\vec{k}}{2\pi}$, $\vec{S}' = \frac{\vec{k}'}{2\pi}$ and $\vec{G}^*$= reciprocal lattice translation vector

When $\vec{G}^* \neq \vec{S}' - \vec{S}$, diffraction occurs due to "shape effect".