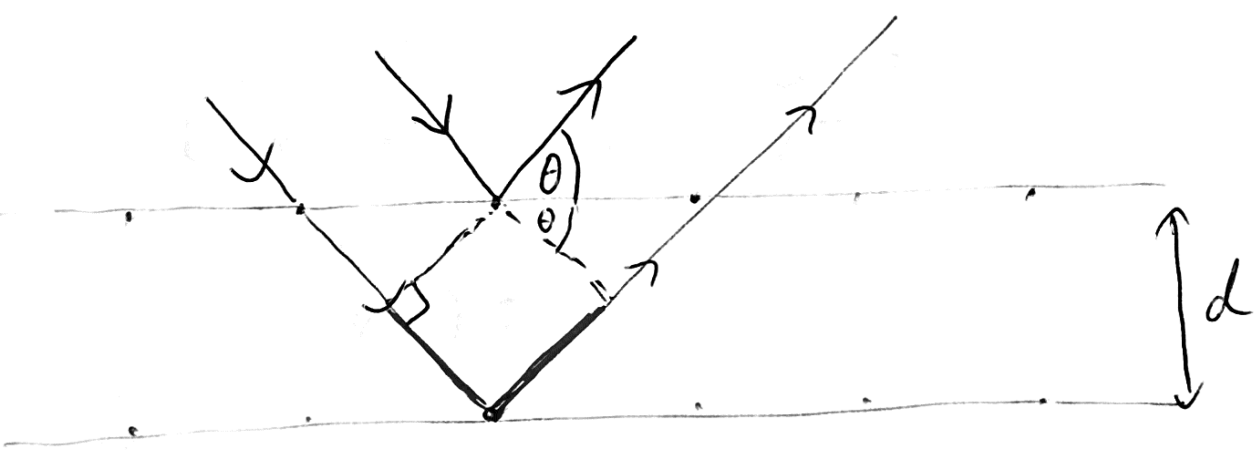
$$\tilde{V}(\vec{k}-\vec{k}') = \frac{(2\pi)^3}{V_{\substack{unit\\cell}}} \sum_{\vec{G}} \delta(\vec{k}-\vec{k}'-\vec{G})\, S(\vec{G})$$

1. scattering is 0 unless $\boxed{\vec{k}-\vec{k}'=\vec{G}}$

Laue condition

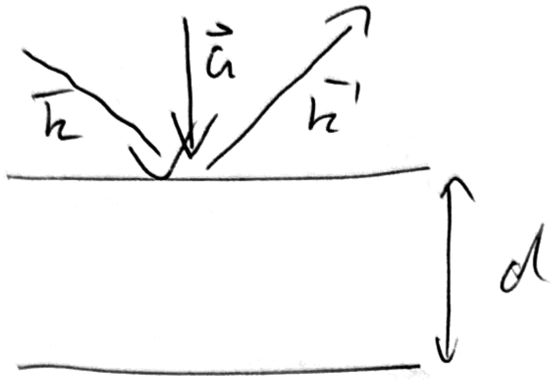
2. Intensity of scattering is $|S(\vec{G})|^2$
with structure factor $S(\vec{G})$



additional distance: $2d\sin\theta$

constructive interference: $\boxed{n\lambda = 2d\sin\theta}$

Bragg condition



define unit vectors: $\hat{k}, \hat{k}', \hat{G}$

$$\hat{k} \cdot \hat{G} = \sin\theta$$

$$\hat{k}' \cdot \hat{G} = -\sin\theta$$

$$\bar{k} = \left(\frac{2\pi}{\lambda}\right)\hat{k}$$

assume Laue condition: $\vec{k} - \vec{k}' = \vec{G}$

$$\frac{2\pi}{\lambda}(\hat{k} - \hat{k}') = \bar{G}$$

$$\frac{2\pi}{\lambda}(\hat{G}\cdot\hat{k} - \hat{G}\cdot\hat{k}') = \hat{G}\cdot\bar{G}$$

$$\frac{2\pi}{\lambda}(\sin\theta - (-\sin\theta)) = |\vec{G}|$$

$$\frac{2\pi}{|\vec{G}|} 2\sin\theta = \lambda$$

$$d = \frac{2\pi}{|G_{min}|} \rightarrow 2d \sin\theta = n\lambda$$

$$\vec{G} = n \vec{G}_{min}$$

$$S(\vec{G}) = \sum_{\substack{\text{atoms} \\ \alpha}} e^{i\vec{G}\vec{r}} \underbrace{f_\alpha(\vec{G})}_{\text{atomic form factor}}$$

$$= \sum_{\alpha} e^{2\pi i(hu_\alpha + kv_\alpha + lw_\alpha)} f_\alpha(hkl)$$

(hkl) Miller index of $\vec{G}$

$[u_\alpha, v_\alpha, w_\alpha]$ position of atom α in unit cell.

Example 1: CsCl, simple cubic, Cs [0,0,0]
Cl [1/2, 1/2, 1/2]

$$S_{hkl} = f_{Cs} + f_{Cl} e^{2\pi i (h\frac{1}{2} + k\frac{1}{2} + l\frac{1}{2})}$$

$$= f_{Cs} + f_{Cl} (-1)^{h+k+l}$$

Example 2: Cs, bcc
Cs [0,0,0]
Cs [1/2, 1/2, 1/2]

$$S_{hkl} = f_{Cs} + f_{Cs} (-1)^{h+k+l}$$

$$= f_{Cs} \left[1 + (-1)^{h+k+l} \right]$$

vanishes unless $h+k+l$ is even
(selection rule / systematic absence)

for fcc: S vanishes unless h, k, l are all even or all odd

$\{hkl\}$	$N = h^2+k^2+l^2$	sc	bcc	fcc
$\{100\}$	1	✓	×	×
$\{110\}$	2	✓	✓	×
$\{111\}$	3	✓	×	✓
$\{200\}$	4	✓	✓	✓

for sc: $N = 1, 2, 3, 4, 5, 6, 8$

bcc: $N = 2, 4, 6, 8 \ldots$

fcc: $N = 3, 4, 8, 11, 12, 16$