

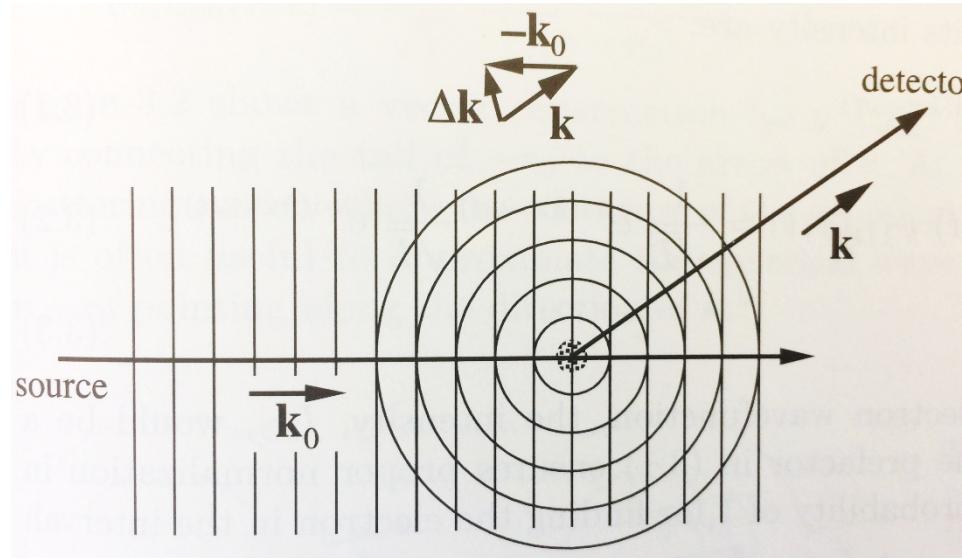
MEAM/MSE 507

Fundamentals of Materials

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Week 5, Lecture 4: Reciprocal space and diffraction patterns
Asynchronous

Interference of wavelets



A **phase factor**, associated with a particular wavelet, can be defined: $e^{-i\Delta\mathbf{k}\cdot\mathbf{R}}$

This has the form of a plane wave but is not a wave. It can be used to determine whether there is constructive or destructive interference when two or more wavelets are scattered from different points in space (defining the set of vectors $\{\mathbf{R}_j\}$):

$$\psi_{phf}(\Delta\mathbf{k}) = \sum_{\{\mathbf{R}_j\}} e^{-i\Delta\mathbf{k}\cdot\mathbf{R}_j}$$

The diffracted wave

Where should we expect to find diffraction? Where the sum of wavelets is maximal:

$$\psi_{max} \propto \text{Max} \left(\sum_{\mathbf{R}} e^{-i\Delta\mathbf{k} \cdot \mathbf{R}} \right)$$

Assuming the primitive translation vectors associated with our unit cell are \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 (and that we have exactly one atom located at each lattice point), then the locations of the atoms can be expressed:

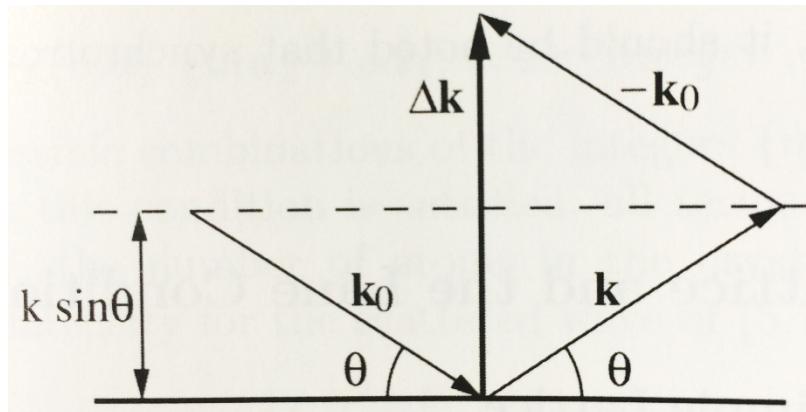
$$\mathbf{R} = m\mathbf{a}_1 + n\mathbf{a}_2 + o\mathbf{a}_3$$

for integers m , n , and o . The sum which we need to maximize then becomes:

$$\begin{aligned} \sum_{\mathbf{R}} e^{-i\Delta\mathbf{k} \cdot \mathbf{R}} &= \sum_{\mathbf{R}} e^{-i\Delta\mathbf{k} \cdot (m\mathbf{a}_1 + n\mathbf{a}_2 + o\mathbf{a}_3)} \\ &= \sum_m \sum_n \sum_o e^{-i\Delta\mathbf{k} \cdot (m\mathbf{a}_1 + n\mathbf{a}_2 + o\mathbf{a}_3)} \end{aligned}$$

and the first term of this sum is $e^0=1$ (corresponding to $m=n=o=0$).

Atom-specific “intrinsic scattering factors” f



The **scattering vector ($\Delta\mathbf{k}$)** is always normal to the diffracting planes.

Notice that it also encompasses the tilt information (θ).

If the atoms are different from one another, they possess different atomic potentials and therefore have different **intrinsic scattering factors f** . This gives the following for the diffracted wave (summing over all wavelet contributions):

$$\psi(\Delta\mathbf{k}) = \sum_{j=1}^N f(\mathbf{R}_j) e^{-i\Delta\mathbf{k} \cdot \mathbf{R}_j}$$

The diffracted wave is proportional to the Fourier transform of the scattering factor distribution in the material.

Diffracted beam intensity

- Not all peaks have the same intensities
- Related to scattering power of different atoms & structure
- The intensity scales as: $I_{hkl} \propto F_{hkl}^2$

where g is a geometric factor, s is a scale factor related to the beam intensity and F is the structure factor

- The structure factor is

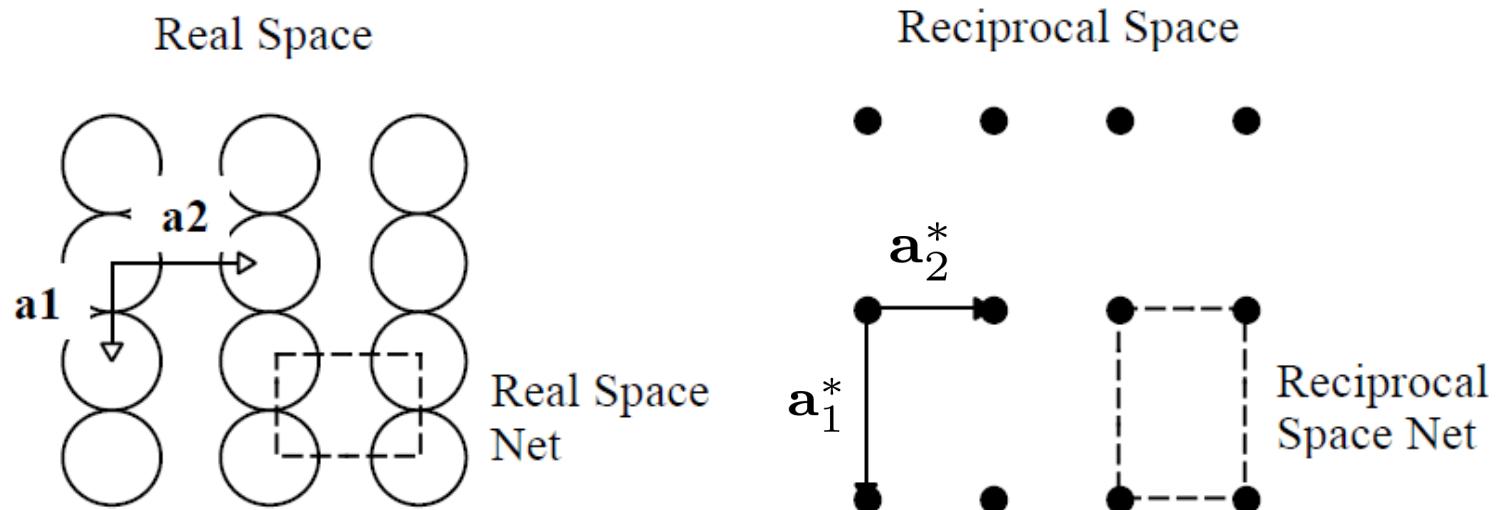
$$\begin{aligned}
 F_{hkl} &= \sum_n f_n \exp[i2\pi\Delta\mathbf{k} \cdot \mathbf{Q}] = \sum_n f_n \exp\left[i\left(\frac{2\pi}{a}\right)(hx_n + ky_n + lz_n)\right] \\
 &= \sum_n f_n \left\{ \cos\left[\left(\frac{2\pi}{a}\right)(hx_n + ky_n + lz_n)\right] + i \sin\left[\left(\frac{2\pi}{a}\right)(hx_n + ky_n + lz_n)\right] \right\}
 \end{aligned}$$

Where do diffraction points occur and what are their relative brightness?

where the sum is over all atoms in the unit cell and f_n is the scattering strength of atom n

Reciprocal lattice (FCC)

FCC(110):



$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$

$$\mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot \mathbf{a}_3 \times \mathbf{a}_1}$$

$$\mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot \mathbf{a}_1 \times \mathbf{a}_2}$$

$$\mathbf{a}_1^* \perp \mathbf{a}_2 \text{ and } \mathbf{a}_2^* \perp \mathbf{a}_1$$

α (angle between \mathbf{a}_1 and \mathbf{a}_1^* is 0°), $\text{Cos}\alpha=1$

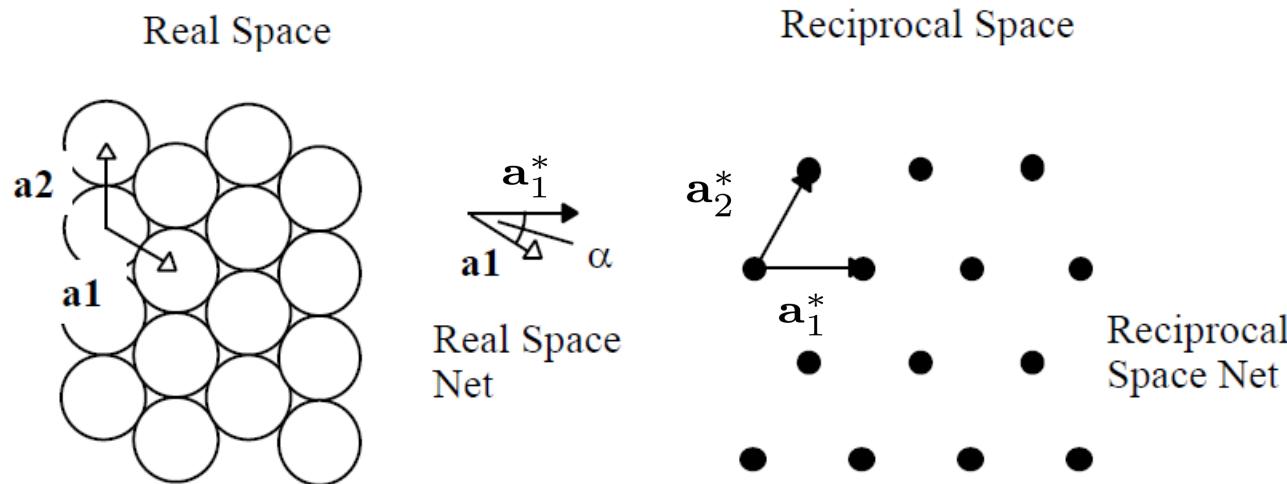
$$\mathbf{a}_1 \cdot \mathbf{a}_1^* = 1$$

$$|\mathbf{a}_1 \times \mathbf{a}_1^*| \text{Cos}\alpha = 1$$

$$|\mathbf{a}_1| = \frac{1}{|\mathbf{a}_1^*|}$$

Reciprocal lattice (FCC)

FCC(111):



\mathbf{a}_1^* not $\perp \mathbf{a}_2$ and \mathbf{a}_2^* not $\perp \mathbf{a}_1$

α (angle between \mathbf{a}_1 and \mathbf{a}_1^* is 30°), $\text{Cos}\alpha = \sqrt{3}/2$

$$\mathbf{a}_1 \cdot \mathbf{a}_1^* = 1$$

$$|\mathbf{a}_1 \times \mathbf{a}_1^*| \text{Cos}\alpha = 1$$

$$|\mathbf{a}_1 \times \mathbf{a}_1^*| \frac{\sqrt{3}}{2} = 1$$

$$|\mathbf{a}_1| = \frac{2}{\sqrt{3}} \frac{1}{|\mathbf{a}_1^*|}$$

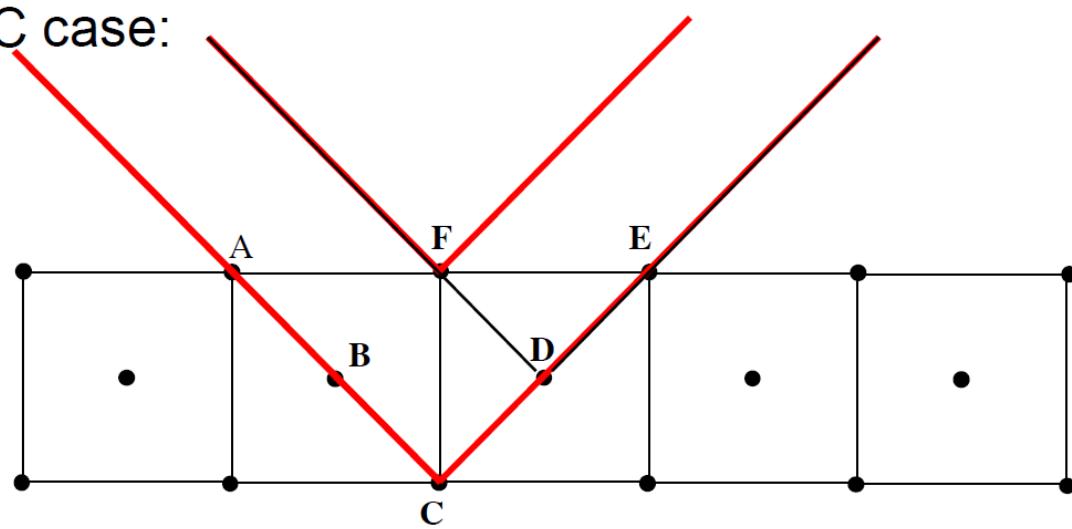
$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$

$$\mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot \mathbf{a}_3 \times \mathbf{a}_1}$$

$$\mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot \mathbf{a}_1 \times \mathbf{a}_2}$$

Non-primitive systematic absences

- When the lattice type is not primitive, some planes yield destructive interference where the primitive cell would have constructive interference
- Consider this BCC case:



- If it were simple cubic, would get (100) reflection if $n\lambda = BC + CD$
- However, if we get constructive interference from the 1st and 3rd plane, we necessarily get destructive interference from the 2nd plane → missing reflection

Structure factor BCC

- The structure factor is

$$F_{hkl} = \sum_n f_n \exp\left[i\left(\frac{2\pi}{a}\right)(hx_n + ky_n + lz_n)\right]$$

- Sum over all atoms in the unit cell
- BCC:** $\mathbf{r}_1=0$, $\mathbf{r}_2=(a/2)(\mathbf{x}+\mathbf{y}+\mathbf{z})$

$$\begin{aligned}
 F_{hkl} &= \sum_n f_n \exp\left[i\left(\frac{2\pi}{a}\right)(hx_n + ky_n + lz_n)\right] \\
 &= f_1 \exp\left[i\left(\frac{2\pi}{a}\right)(h0 + k0 + l0)\right] + f_2 \exp\left[i\left(\frac{2\pi}{a}\right)\left(\frac{a}{2}\right)(h1 + k1 + l1)\right] \\
 &= f_1 \exp[0] + f_2 \exp[i\pi(h+k+l)] \\
 &= f_1 + f_2 (\exp[i\pi])^{(h+k+l)} = f_1 + f_2 (-1)^{(h+k+l)} = f \left[1 + (-1)^{(h+k+l)} \right] \\
 &= \begin{cases} 2f & h+k+l \text{ even} \\ 0 & h+k+l \text{ odd} \end{cases}
 \end{aligned}$$

Structure factor FCC

$$F_{hkl} = \sum_n f_n \exp \left[i \left(\frac{2\pi}{a} \right) (hx_n + ky_n + lz_n) \right]$$

- FCC: $\mathbf{r}_1=0$, $\mathbf{r}_2=(a/2)(\mathbf{x}+\mathbf{y})$, $\mathbf{r}_3=(a/2)(\mathbf{y}+\mathbf{z})$, $\mathbf{r}_4=(a/2)(\mathbf{z}+\mathbf{x})$

$$\begin{aligned}
 F_{hkl} &= \sum_n f_n \exp \left[i \left(\frac{2\pi}{a} \right) (hx_n + ky_n + lz_n) \right] \\
 &= f_1 \exp[0] + f_2 \exp[i\pi(h+k)] + f_3 \exp[i\pi(k+l)] + f_4 \exp[i\pi(l+h)] \\
 &= f_1 + f_2 (\exp[i\pi])^{h+k} + f_3 (\exp[i\pi])^{k+l} + f_4 (\exp[i\pi])^{l+h} \\
 &= f_1 + f_2(-1)^{h+k} + f_3(-1)^{k+l} + f_4(-1)^{l+h} = f [1 + (-1)^{h+k} + (-1)^{k+l} + (-1)^{l+h}]
 \end{aligned}$$

$$F_{hkl} = \begin{cases} 4f, & h, k, l \text{ all even or all odd} \\ 0, & h, k, l \text{ mixed parity} \end{cases}$$

Non-primitive systematic absences

- Translational symmetry elements and their systematic absenses
- Also see International Tables of Crystallography

Symmetry element	Affected reflection	Condition for systematic absence
Body-centered (I)	hkl	h+k+l is odd
A-face centered	hkl	k+l is odd
B-face centered	hkl	h+l is odd
C-face centered	hkl	h+k is odd
Face centered (F)	hkl	h, k, l have mixed parity (i.e., not all even or all odd)
Screw axis 2_1 along a	h00	h is odd
Screw axis 2_1 along b	0k0	k is odd
Screw axis 2_1 along c	00l	l is odd
Glide plane $\perp b$, $a/2$ translation	h0l	h is odd