EEE 6212
Semiconductor Materials

Lecture 4: The reciprocal lattice

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- definition of reciprocal lattice
- relation to Fourier transform
- Wigner-Seitz cell
- 1st Brillouin zone
- diffraction by slit and grating
- Bragg's law
- Ewald's sphere
- structure factors
- diffraction (spot) patterns

Definition of reciprocal lattice

Definition:

Given a set of points $\underline{\boldsymbol{R}}$ constituting a Bravais lattice and a plane wave of form exp (2π i$\underline{\boldsymbol{k}}\underline{\boldsymbol{r}}$), the set of all wave vectors $\underline{\boldsymbol{K}}$ that yield plane waves with the periodicity of the given Bravais lattice is know as its reciprocal lattice, i.e.:

exp [2πi $\underline{\boldsymbol{K}}$($\underline{\boldsymbol{r}}$+$\underline{\boldsymbol{R}}$)]=exp ($2\pi$i $\underline{\boldsymbol{K}}\underline{\boldsymbol{r}}$) for all $\underline{\boldsymbol{r}}$

→ exp (2πi $\underline{\boldsymbol{K}}\underline{\boldsymbol{R}}$)=1

Relation to Fourier transform

remember:

This is similar to a Fourier transform from real space ($\underline{\boldsymbol{r}}$) to $\underline{\boldsymbol{k}}$-space where

$$F(\underline{\boldsymbol{k}}) = \int f(\underline{\boldsymbol{r}}) \exp(2\pi i\, \underline{\boldsymbol{k}}\underline{\boldsymbol{r}})\, d^3r$$

describes the function of all spatial frequencies that the function $f(\underline{r})$ is made up of.

Construction of reciprocal lattice

Let $\underline{\boldsymbol{a}}=\underline{\boldsymbol{a}}_1, \underline{\boldsymbol{b}}=\underline{\boldsymbol{a}}_2, \underline{\boldsymbol{c}}=\underline{\boldsymbol{a}}_3$ be the unit cell vectors of the direct Bravais lattice.

The reciprocal lattice can then be generated by

$$\underline{\boldsymbol{b}}_i = \varepsilon_{ijk} (\underline{\boldsymbol{a}}_j \times \underline{\boldsymbol{a}}_k)/[\underline{\boldsymbol{a}}_i \cdot (\underline{\boldsymbol{a}}_j \times \underline{\boldsymbol{a}}_k)]$$

where ε_{ijk}=+1if i,j,k are a cyclic and = –1 if anti-cyclic permutation of the sequence (1,2,3).

Note then $\underline{\boldsymbol{b}}_i \cdot \underline{\boldsymbol{a}}_j = \delta_{ij}$ = 0, if i≠j and =1 if i=j. Hence, for any $\underline{\boldsymbol{k}} = k_1\underline{\boldsymbol{b}}_1 + k_2\underline{\boldsymbol{b}}_2 + k_3\underline{\boldsymbol{b}}_3$ and a Bravais lattice vector $\underline{\boldsymbol{R}} = n_1\underline{\boldsymbol{a}}_1 + n_2\underline{\boldsymbol{a}}_2 + n_3\underline{\boldsymbol{a}}_3$, if follows $\underline{\boldsymbol{k}}\,\underline{\boldsymbol{R}} = k_1n_1 + k_2n_2 + k_3n_3$ is an integer, hence exp $(2\pi i\, \underline{\boldsymbol{k}}\,\underline{\boldsymbol{R}})$=1.

So, the reciprocal lattice is itself a Bravais lattice!

Construction of reciprocal lattice

If the lattice is *cubic primitive* with

$\underline{\boldsymbol{a}}_1 = a\hat{\underline{\boldsymbol{x}}}$, $\underline{\boldsymbol{a}}_2 = a\hat{\underline{\boldsymbol{y}}}$, $\underline{\boldsymbol{a}}_3 = a\hat{\underline{\boldsymbol{z}}}$,

then the reciprocal lattice is simply given by

$\underline{\boldsymbol{b}}_1 = 1/a\ \hat{\underline{\boldsymbol{x}}}$, $\underline{\boldsymbol{b}}_2 = 1/a\ \hat{\underline{\boldsymbol{y}}}$, $\underline{\boldsymbol{b}}_3 = 1/a\ \hat{\underline{\boldsymbol{z}}}$

That's *easy*.

For more complicated lattices, it is useful to construct suitable **primitive unit cells** which contain always only exactly 1 single atom. This involves creating smaller unit cells that are of lower symmetry, e.g. are no longer cubic for bcc and fcc.

Construction of primitive lattice *for bcc*

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}). \qquad (4.3)$$

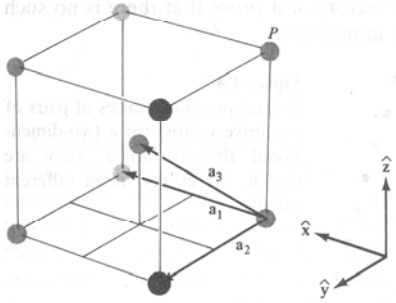


Figure 4.6
Three primitive vectors, specified in Eq. (4.3), for the body-centered cubic Bravais lattice. The lattice is formed by taking all linear combinations of the primitive vectors with integral coefficients. The point P, for example, is $P = -\mathbf{a}_1 - \mathbf{a}_2 + 2\mathbf{a}_3$.

from: Neil W. Ashcroft & N. David Mermin: Solid State Physics, CBS Publ., 1988

Construction of another primitive lattice *for bcc*

A more symmetric set (see Figure 4.7) is

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}). \qquad (4.4)$$

It is important to convince oneself both geometrically and analytically that these sets do indeed generate the bcc Bravais lattice.

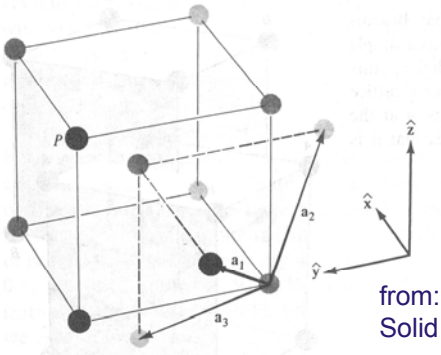


Figure 4.7
A more symmetric set of primitive vectors, specified in Eq. (4.4), for the body-centered cubic Bravais lattice. The point P, for example, has the form $P = 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

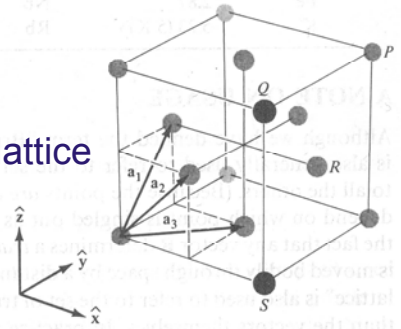
from: Neil W. Ashcroft & N. David Mermin: Solid State Physics, CBS Publ., 1988

Construction of reciprocal lattice for *fcc*

A symmetric set of primitive vectors for the face-centered cubic lattice (see Figure 4.9) is

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \tag{4.5}$$

Figure 4.9
A set of primitive vectors, as given in Eq. (4.5), for the face-centered cubic Bravais lattice. The labeled points are $P = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$, $Q = 2\mathbf{a}_2$, $R = \mathbf{a}_2 + \mathbf{a}_3$, and $S = -\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.



This yields as reciprocal lattice

$\underline{\boldsymbol{b}}_1 = 1/a\ (\underline{\boldsymbol{y}} + \underline{\boldsymbol{z}} - \underline{\boldsymbol{x}})$,

$\underline{\boldsymbol{b}}_2 = 1/a\ (\underline{\boldsymbol{z}} + \underline{\boldsymbol{x}} - \underline{\boldsymbol{y}})$,

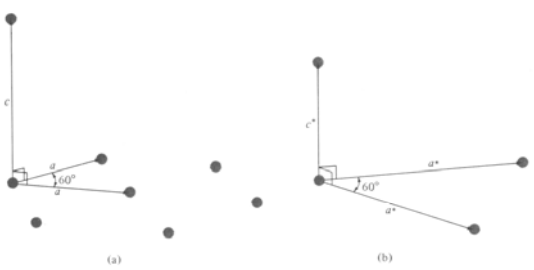
$\underline{\boldsymbol{b}}_3 = 1/a\ (\underline{\boldsymbol{x}} + \underline{\boldsymbol{y}} - \underline{\boldsymbol{z}})$.

This describes a bcc lattice of unit cell size $2/a$.

Construction of reciprocal lattice for *bcc* and *hcp*

If the reciprocal lattice of an fcc lattice of unit cell size a is a bcc lattice of unit cell size $2/a$, then, by reciprocity, the reciprocal lattice of a bcc must be fcc with a unit cell size of $1/(2a)$.

The reciprocal lattice (b) of hcp lattice (a) is a simple hexagonal lattice with lattice constants of $2/(\sqrt{3}a)$ and $1/c$, rotated through 30° about the $\underline{\boldsymbol{c}}$-axis, as shown.

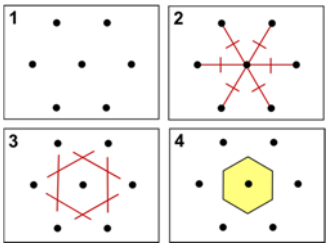


from: Neil W. Ashcroft & N. David Mermin: Solid State Physics, CBS Publ., 1988

Wigner-Seitz cell

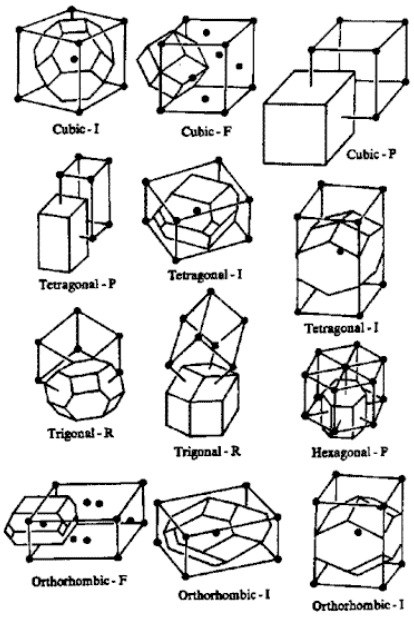
Pick any lattice point. Then, lines are drawn to all nearby (closest) lattice points. At the midpoint of each line, a plane is drawn perpendicular to each of the first set of lines.
By using this method, the smallest volume that can be attributed to a lattice point is enclosed and is called the **Wigner–Seitz primitive cell**. All space within the lattice will be filled by this type of primitive cell and will leave no gaps.

in 2D:



Wigner-Seitz cell

in 3D:
For each of the 14 Bravais lattices there is a least one Wigner-Seitz cell. If different ratios of the crystal axes are considered, there are 24 distinct forms of Wigner-Seitz cells; half of which are illustrated to the right.
credit: Laura Malcolm, March 1997

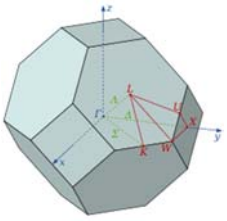


1st Brillouin zone

Definition:
The Wigner-Seitz primitive cell of the reciprocal lattice is called the first Brillouin zone.
Hence, the 1st Brillouin zone always refers to reciprocal space. As the reciprocal of the bcc lattice is fcc, the 1st Brillouin zone of the bcc lattice is just the fcc Wigner-Seitz cell, and vice versa.

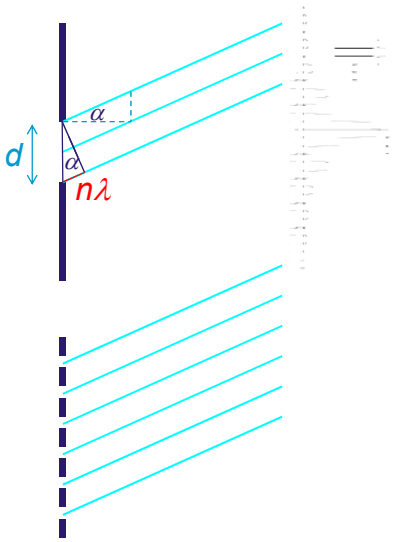
Figure 5.2
(a) The first Brillouin zone for the body-centered cubic lattice. (b) The first Brillouin zone for the face-centered cubic lattice.

(a) bcc



(b) fcc

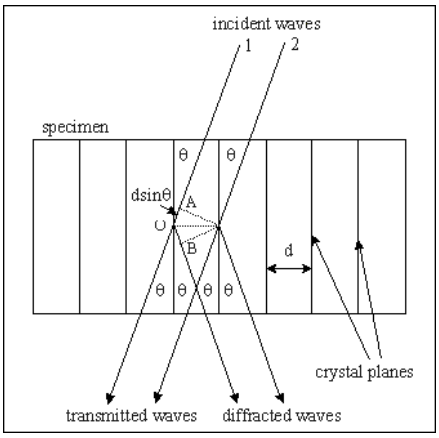
Diffraction by slit and grating



Principle: divide slit into an even number of sections whose contributions cancel pairwise, leading to extinction, due to deconstructive interference, for the single slit if $\sin\alpha = n\lambda/d$
where $n \in N$ and λ=wavelength

For the grating of period d, the same formula gives the maxima due to constructive interference.

Bragg's Law



optical path difference between diffracted waves 1 and 2 is $2d \sin\theta$.

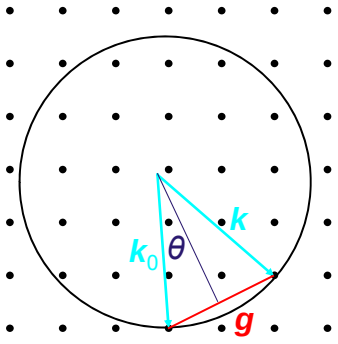
If $2d \sin\theta = n\lambda$ then the waves are in-phase and interference with each other constructively;

therefore the conditions for diffraction is:

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

BRAGG'S LAW

Ewald's sphere construction



construct so-called 'reciprocal lattice' with points of all crystal reflections, then draw circle with radius $k_0=1/\lambda$ and determine the directions for the incoming beam $\boldsymbol{k}_0$ and the scattered beam $\boldsymbol{k}$. Diffraction then occurs only if difference is a reciprocal lattice point, i.e.:

$\sin\theta = n(g/2)/\ k_0=n\lambda/2d$

same result as Bragg's Law!

The structure factor (kinematical diffraction theory)

The wavefunction of a diffracted wave in the Born (i.e. high energy) approximation by a crystal potential $V(\boldsymbol{r})$ is given by the following formula wherein $\Delta\boldsymbol{k}=\boldsymbol{k}_0-\boldsymbol{k}$ with $\Delta k=2\sin\theta/\lambda$:

$\Psi_s(\boldsymbol{k},\boldsymbol{r})= A_0$ amplitude of ingoing wave

$\bullet\ \exp(2\pi i\boldsymbol{kr})/r$ spherical wave generated

$\bullet\ \Sigma_n \exp(-2\pi i\Delta\boldsymbol{kr}_n)$ sum over all unit cells

$\bullet\ \Sigma_m \exp(-2\pi i\Delta\boldsymbol{kr}_m)\ 2\pi m_0 e h^{-2}\,\Sigma_{atom} V(\boldsymbol{r}_j)\exp(-2\pi i\Delta\boldsymbol{kr}_i)\,d\tau_j$

$f_m(\theta)$: atomic scattering factor (tabulated)

$\boldsymbol{F_n(\theta)}$: **structure factor** (can be easily calculated)

The structure factor (kinematical diffraction theory)

example:

The structure factors of the sphalerite structure.

$F_n(\theta) = \Sigma_m \exp(-2\pi i\Delta\boldsymbol{kr}_m)\, f_m(\theta)$

Take $\underline{\boldsymbol{r}}_m=(u_m,v_m,w_m)$ as coordinates of the mth atom in the unit cell.

group-III atoms at: (0,0,0), (½,½,0), (½,0,½), (0,½,½)

group-V atoms at: (¼,¼,¼), (¼,¾,¾), (¾,¼,¾), (¾,¾,¼)

Looking along <100> zone axis, the projected unit cell is mirror symmetric so that in $\exp(-2\pi i\Delta\boldsymbol{kr}_m)=\cos(2\pi i\Delta\boldsymbol{kr}_m) - i\sin(2\pi i\Delta\boldsymbol{kr}_m)$ all the sin terms cancel, so:

$F_n(\theta)=\Sigma_m \cos[2\pi i(hu_m+kv_m+\ell w_m)]\, f_m(\theta)=$

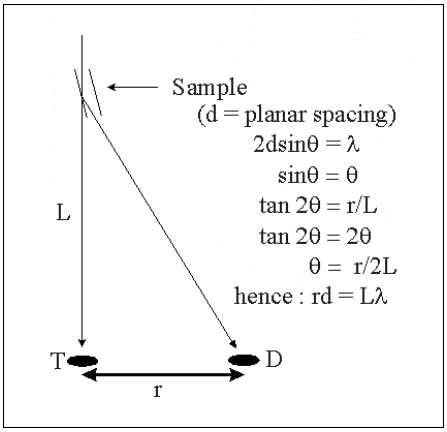
- $4(f^2_{III}+f^2_V)^{1/2}$ if h,k,ℓ all odd
- $4(f_{III}+f_V)$ if h,k,ℓ even and *
- $4(f_{III}-f_V)$ if h,k,ℓ even and **
- 0 if h,k,ℓ mixed

*h+k+ℓ=4n, ** h+k+ℓ=4n+2

remember:

intensity $\propto |F_{hkl}|^2$ and $F(\theta) \propto Z\sin^{-2}(\theta)$

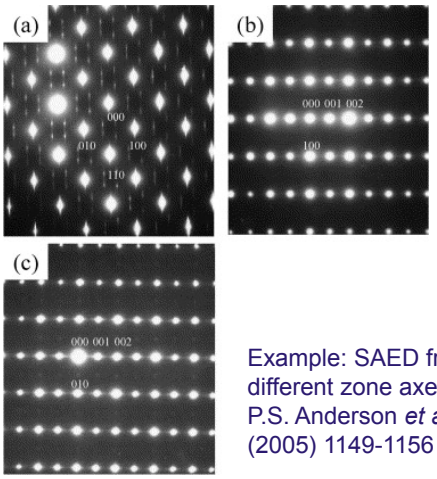
Spot diffraction patterns



Each set of lattice planes near the Bragg condition gives a **point** in the diffraction pattern.

The spacing "*r*" in the diffraction pattern of back focal plane is *inversely* proportional to the real crystallographic interplanar spacing "*d*" because their product is a constant, namely the product of camera length *L* and wavelength λ.

Space group determination from tilting experiments



Principle: take diffraction patterns from various directions, then try to index the spot patterns and find forbidden reflections (*F*=0)

Example: SAED from $NdBaCo_2O_{5.5}$ along three different zone axes: <100>, <010>, <001>
P.S. Anderson *et al*., Sol. State Sciences 7 (2005) 1149-1156

Summary 1/2

- The reciprocal lattice $\underline{\boldsymbol{K}}$ is defined by $\exp(2\pi i\, \underline{\boldsymbol{K}}\underline{\boldsymbol{R}})=1$ for a Bravais lattice at $\underline{\boldsymbol{R}}$. This is similar to a Fourier transform.
- The reciprocal lattice can be constructed using $\underline{\boldsymbol{b}}_i = \varepsilon_{ijk}\,(\underline{\boldsymbol{a}}_j \times \underline{\boldsymbol{a}}_k)/[\underline{\boldsymbol{a}}_i \cdot (\underline{\boldsymbol{a}}_j \times \underline{\boldsymbol{a}}_k)]$
- The reciprocal lattice is also a Bravais lattice.
- The reciprocal lattice of the reciprocal lattice gives the original lattice (in real space).
- The reciprocal lattice of fcc is bcc, and vice versa.
- The 1st Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice.
- Bragg's law of diffraction states $\sin\theta = n\lambda/(2d)$.
- This is identical to diffraction from an optical grating of spacing d under angle $\alpha=2\theta$ total angle of deflection.

Summary 2/2

- Ewald's sphere construction in reciprocal space yields Bragg's law (and a bit more we have not covered yet…).
- The intensity of a diffraction spot in kinematical approx. is given by $|F_{hkl}|^2$ where $F_n(\theta) = \Sigma_m \exp(-2\pi i \Delta \boldsymbol{kr}_m)\, f_m(\theta)$ sums over all atomic scattering factors with the correct phase term, which is governed by the position of all m atoms within the n^{th} unit cell.
- $F_{hkl}=0$ means the corresponding diffraction spot is kinematically forbidden and hence absent or at least very weak.
- Spot diffraction patterns hence tell is about symmetry, (space group), lattice spacings and angles (reciprocal dimensions) and structure factors.