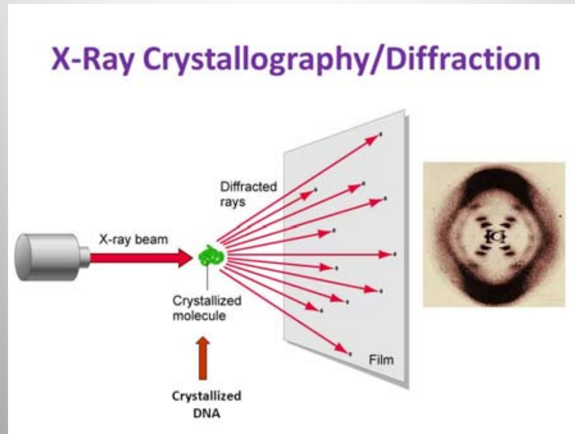


PHYS485

Materials Physics

Dr. Gregory W. Clark
Manchester University

EM Waves and the Lattice

- A plane wave $\tilde{\vec{E}}(\vec{r},t) = \hat{n}\,\tilde{E}_o\, e^{i(\vec{k}\cdot\vec{r}-\omega t)}$ travels through a Bravais lattice (set of points $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$)
- For certain choices of wavevector the wave will have the same periodicity as the lattice.
- The set of all wavevectors $\vec{G} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$ that yield plane waves with the periodicity of the Bravais lattice is known as the **reciprocal lattice**

The Reciprocal Lattice

- Motivation …
- Recall the Fourier Series: any periodic function, f(t), can be expanded in

$$f(t) = \frac{a_o}{2} + \sum_{n=1}^{\infty} [a_n \cos(n\omega t) + b_n \sin(n\omega t)]$$

where
$$a_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\cos(n\omega t)\,dt, \quad n = 0,\, 1,\, 2,\, \ldots$$

$$b_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\sin(n\omega t)\,dt, \quad n = 1,\, 2,\, 3,\, \ldots$$

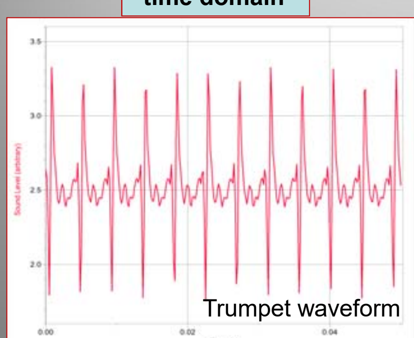
- The Fourier Series can also be written as

$$f(t) = \sum_{n=-\infty}^{\infty} c_n\, e^{in\omega t} = \sum_{n=-\infty}^{\infty} c_n\, e^{i2\pi nt/T}, \quad n = 0,\, \pm 1,\, \pm 2,\, \ldots$$

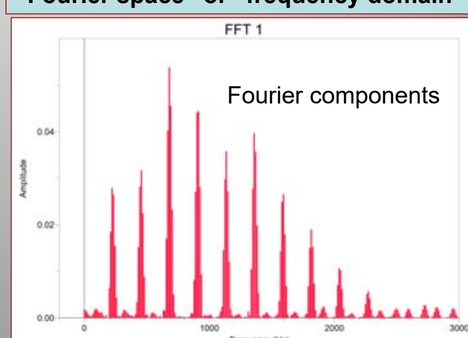
where $c_n = \frac{1}{T}\int_{-T/2}^{T/2} f(t)\, e^{-in\omega t}\, dt$

- One context: **sound**

“time domain”

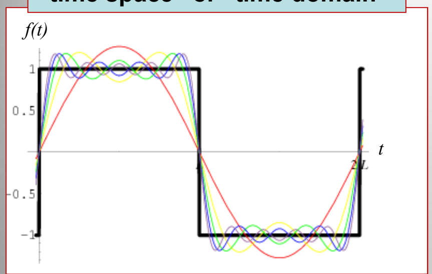


“Fourier space” or “frequency domain”

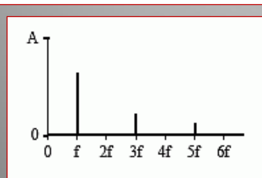


- Other examples:

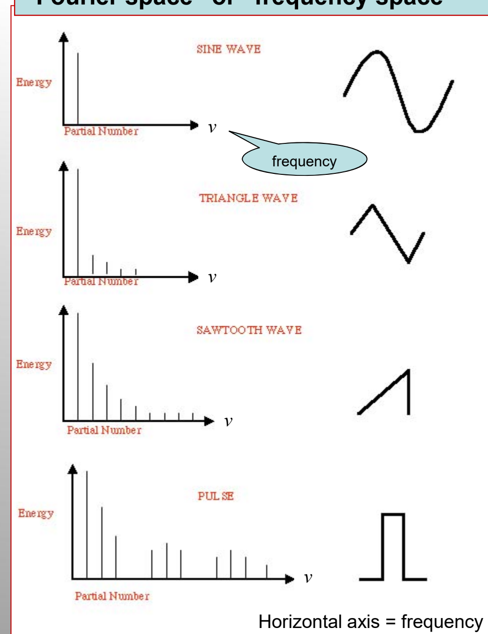
"time space" or "time domain"



$$f(t)=\frac{4}{\pi}\sum_{n=1,3,5,\ldots}^{\infty}\frac{1}{n}\sin\left(\frac{n\pi t}{T}\right)$$



"Fourier space" or "frequency space"



The Lattice

- In a crystal the lattice vectors describe translational symmetry

$$\vec{R}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$$

n affects scattering of photons, neutrons & electrons

- The electron number density is a periodic function

$$n(\vec{r}+\vec{R})=n(\vec{r})$$

- So, <u>in 1-D</u>, we can write

$$n(x)=\sum_p n_p e^{i2\pi px/a}, \quad p=0,\pm1,\pm2,\ldots$$

where $n^*_{-p}=n_p$ and $n_p=\frac{1}{a}\int_0^a n(x)e^{-i2\pi px/a}dx$

The points $2\pi p/a$ are **reciprocal lattice points**

The Reciprocal Lattice

- Since p indexes the *allowed* $2\pi p/a$ values (some have non-zero integrals) we can say that the reciprocal lattice points tell us the *allowed* terms in the Fourier series. A term is allowed if it is consistent with the periodicity of the Xtal!

- In 3-D, we need the set of all vectors, $\vec{G}$, such that

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}}\, e^{i\,\vec{G}\cdot\vec{r}}$$

  is invariant under all Xtal translations.

- The Fourier coefficients determine (X-ray) *scattering amplitude.* Inverting gives

$$n_{\vec{G}} = \frac{1}{V_{cell}} \int_{cell} dV\, n(\vec{r})\, e^{i\,\vec{G}\cdot\vec{r}}$$

Reciprocal Lattice Vectors

- Look at the vectors, $\vec{G}$

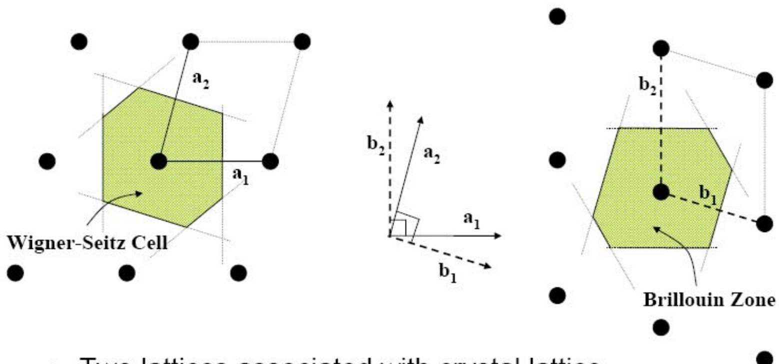
- Construct axis vectors of the reciprocal lattice:

$$\vec{b}_1 = \frac{2\pi\,\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \qquad \vec{b}_2 = \frac{2\pi\,\vec{a}_3\times\vec{a}_1}{\vec{a}_2\cdot(\vec{a}_3\times\vec{a}_1)} \qquad \vec{b}_3 = \frac{2\pi\,\vec{a}_1\times\vec{a}_2}{\vec{a}_3\cdot(\vec{a}_1\times\vec{a}_2)}$$

Note that $\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$

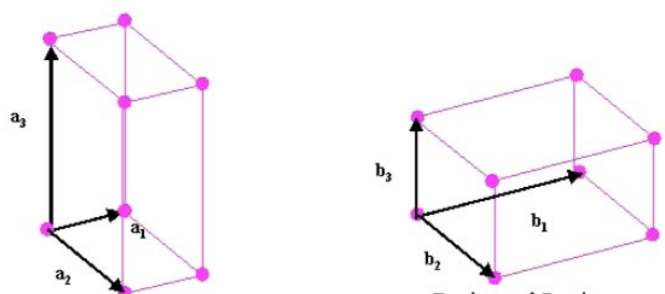
For cubic lattice $\begin{cases} \vec{a}_i = a\,\hat{e}_i \\ \vec{b}_i = \dfrac{2\pi}{a}\hat{e}_i \end{cases}$

Real & Reciprocal lattices in 2 D



- Two lattices associated with crystal lattice
- $\mathbf{b}_1$ perpendicular to $\mathbf{a}_2$, $\mathbf{b}_2$ perpendicular to $\mathbf{a}_1$
- Wigner-Seitz cell of reciprocal lattice called the "First Brillouin Zone" or just "Brillouin Zone"

Three Dimensional Lattices Simplest examples

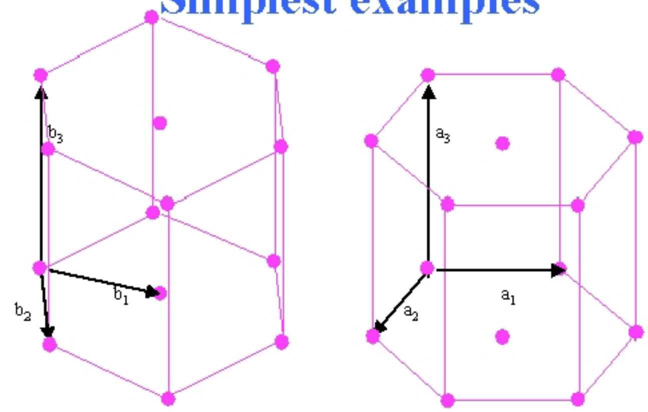


Simple Orthorhombic Bravais Lattice with $a_3 > a_2 > a_1$

Reciprocal Lattice Note: $b_1 > b_2 > b_3$

- **Long lengths in real space imply short lengths in reciprocal space and vice versa**

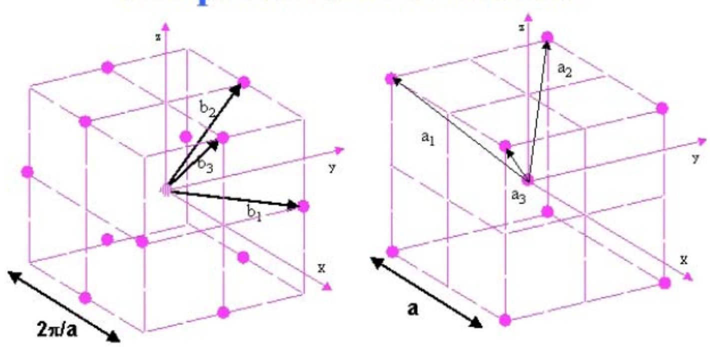
Three Dimensional Lattices
Simplest examples



Reciprocal Lattice

Hexagonal Bravais Lattice

Face Centered - Body Centered Cubic
Reciprocal to one another



Reciprocal lattice is
Face Centered Cubic

Primitive vectors and the
conventional cell of bcc lattice

- Points in the reciprocal lattice are mapped by the reciprocal lattice vectors

$$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

where the m_i are integers.

Note that $\vec{a}_i \cdot \vec{G} = 2\pi\, m_i$

- For example, the SC lattice has

$$\vec{G} = m_1\frac{2\pi}{a}\hat{i} + m_2\frac{2\pi}{a}\hat{j} + m_3\frac{2\pi}{a}\hat{k}$$

- These vectors are the ones in the Fourier series and have the desired X-tal invariance.

Reciprocal Lattice Vectors

- **Theorem:** For any family of lattice planes separated by a distance *d*, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length of $2\pi/d$.

- **Conversely**, for any reciprocal lattice vector, there is a family of lattice planes normal to it and separated by a distance *d*, where $2\pi/d$ is the length of the shortest reciprocal lattice vector parallel to them.

Diffraction with Real Atoms

- The amplitude of a scattered wave is given by

$$\mathrm{A} \propto \left[\sum_R \exp(i\vec{R}\cdot\Delta\vec{k})\right]\left[\sum_p f_{ap}(\theta)\exp(i\vec{r}_p\cdot\Delta\vec{k})\right]$$

or $$A \propto \sum_R e^{i\vec{R}\cdot\vec{G}} S_k$$ for constructive interference

[We'll show this shortly!]

[$\vec{R}$ points to unit cells, $\vec{r}_p$ to atoms in unit cell; $\vec{r}'$ is the integration variable for e- density]

where $$S_{\vec{G}} = \sum_p f_{ap}(\theta)e^{i\vec{G}\cdot\vec{r}_p} = \text{geometric structure factor}$$

$$f_{ap}(\theta) = f_e(\theta)\int_p \rho(\vec{r}')\exp(i\vec{r}'\cdot\Delta\vec{k})d^3\vec{r}'$$

$f_{ap}(\theta)$ is the atomic form factor (atomic scattering function)

$f_e(\theta)$ is the electron form factor (electron scattering function)