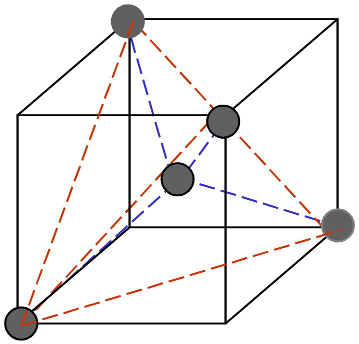
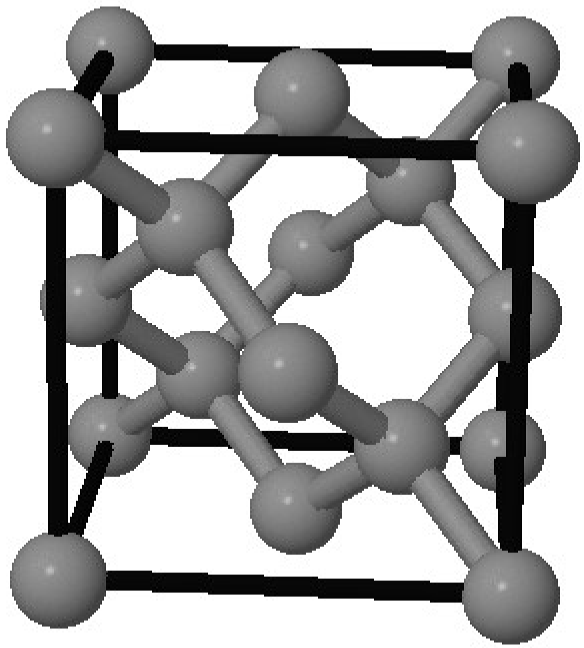
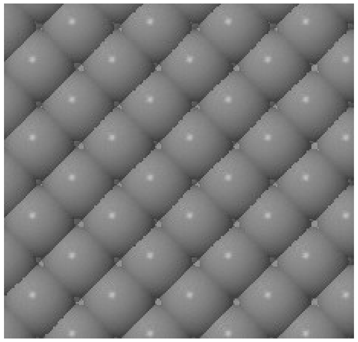
Crystal structure, Fourier Series

Diamond

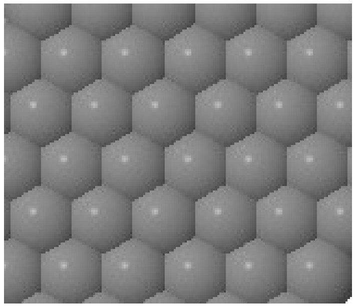


$a = b = c, \quad \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$





(100): $\frac{2}{a^2}$



(111): $\frac{4}{\sqrt{3}a^2}$

Space group: 227
point group: m3m

Primitive lattice vectors:

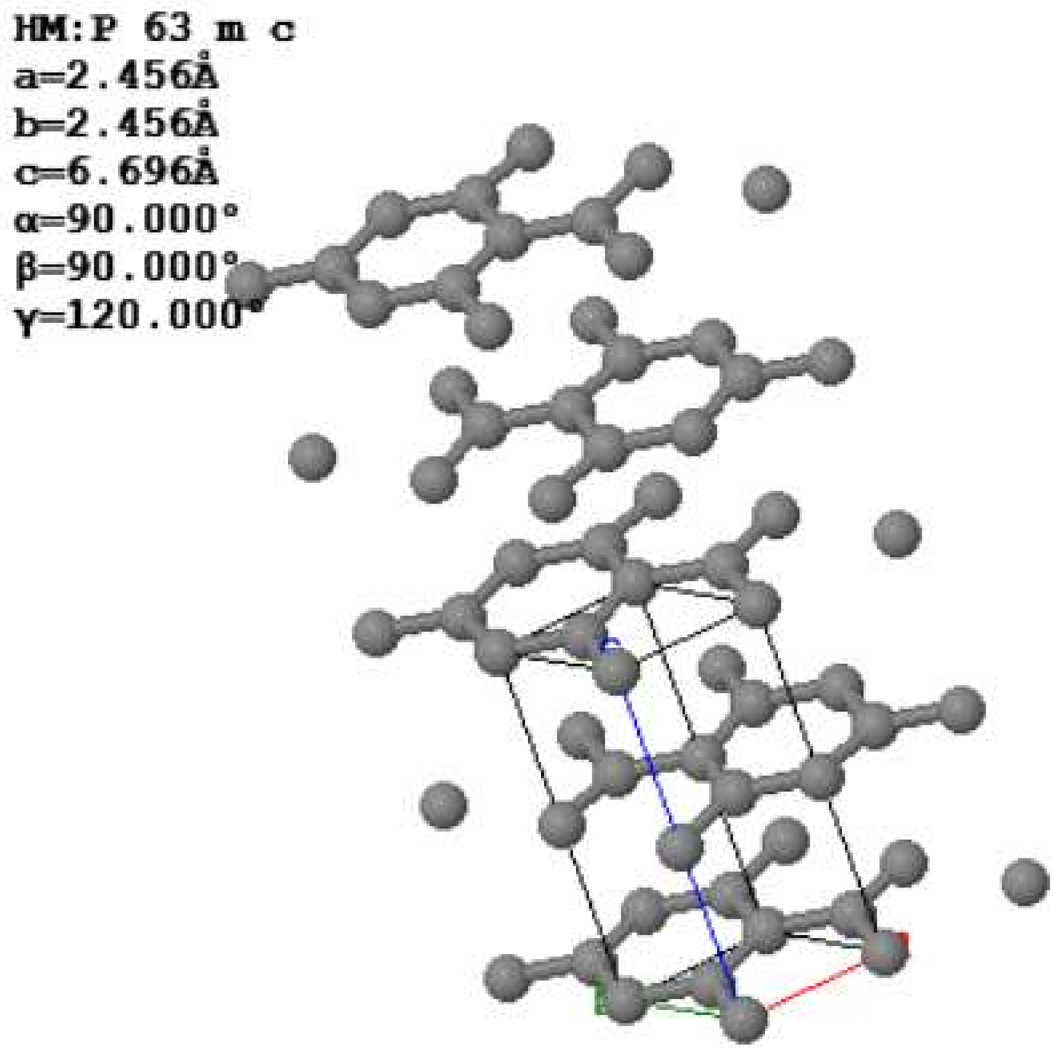
$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}, \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}, \qquad \vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}.$$

Basis: $\vec{B}_1 = (0, 0, 0), \qquad \vec{B}_2 = (0.25, 0.25, 0.25).$

graphite

Space group 194

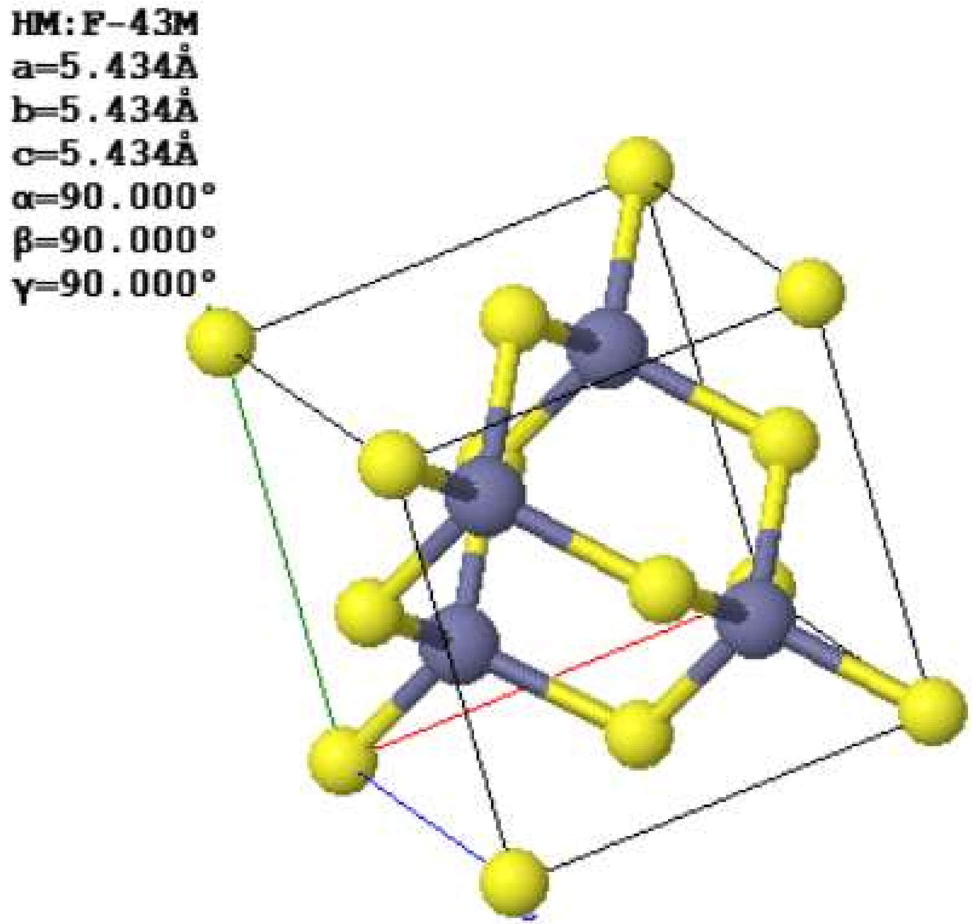
4 inequivalent C atoms in the primitive unit cell



Polytypes of carbon
graphite (hexagonal)
graphene
carbon nanotubes
diamond
rhobohedral graphite
hexagonal diamond

zincblende

ZnS
GaAs
InP

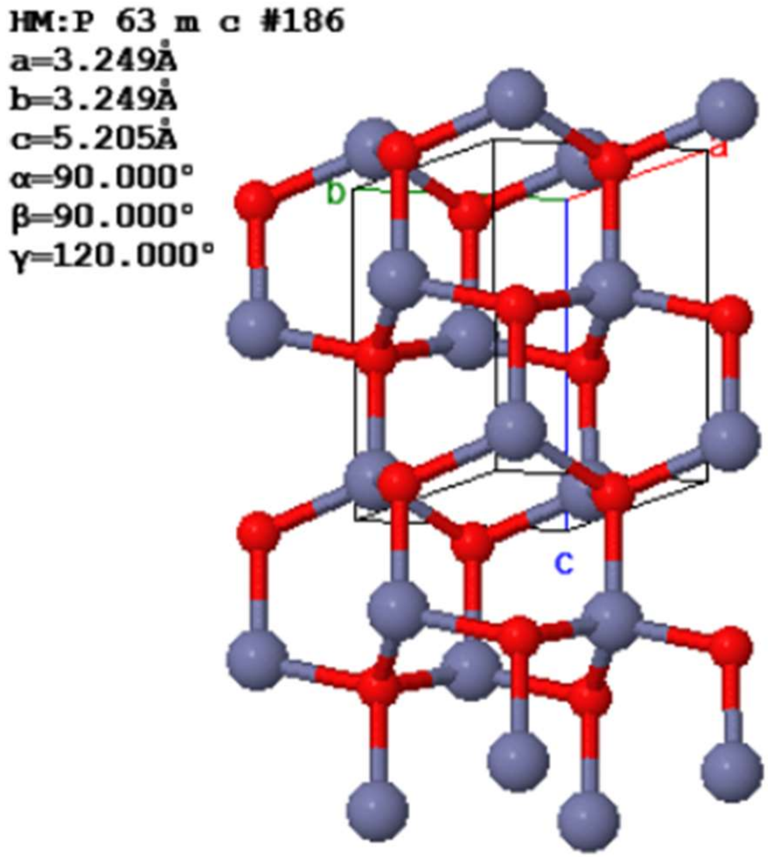


space group 216
$F\bar{4}3m$

wurtzite

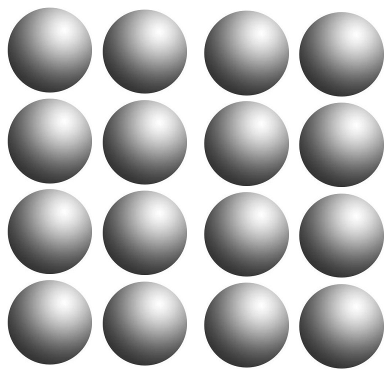
ZnS
ZnO
CdS
CdSe
GaN
AlN

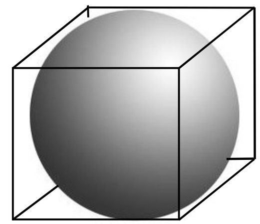
Number 186



There are 2 polytypes of ZnS: zincblende and wurtzite

atomic packing density



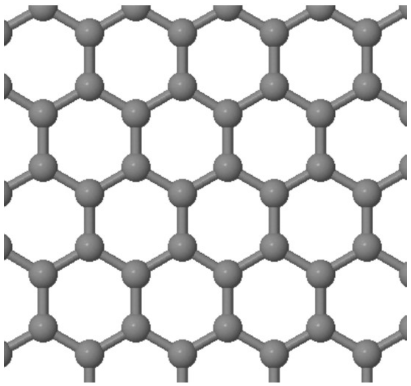


$$\frac{\frac{4}{3}\pi\left(L/2\right)^3}{L^3} = \frac{\pi}{6} \approx 0.52$$

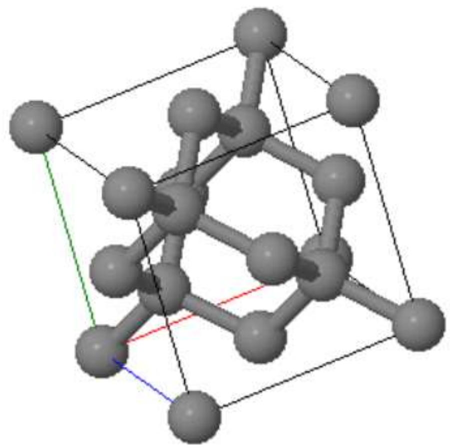
fcc, hcp = 0.74
random close pack = 0.64
simple cubic = 0.52
diamond = 0.34

Coordination number

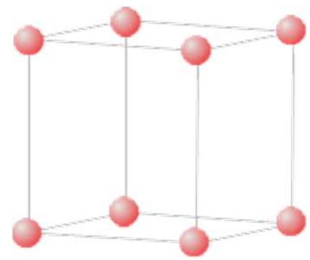
Number of nearest neighbors an atom has in a crystal



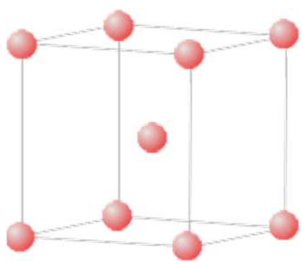
Graphene 3



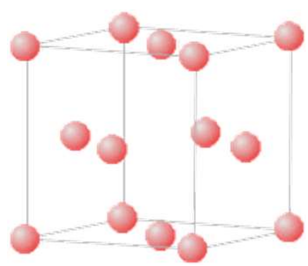
diamond 4



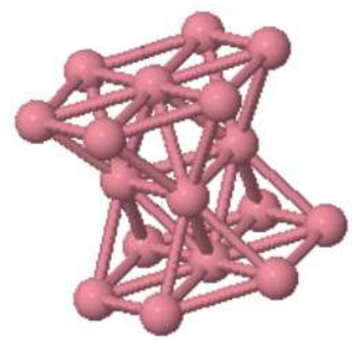
sc 6



bcc 8

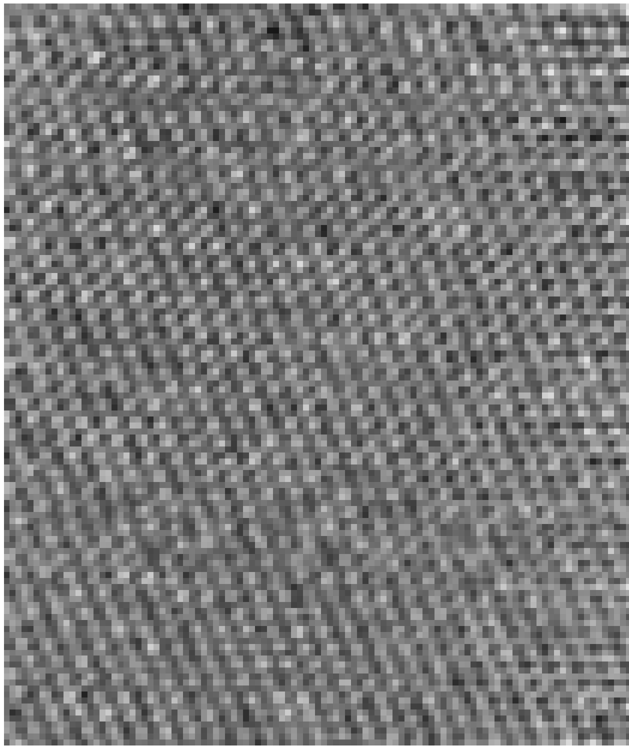


fcc 12

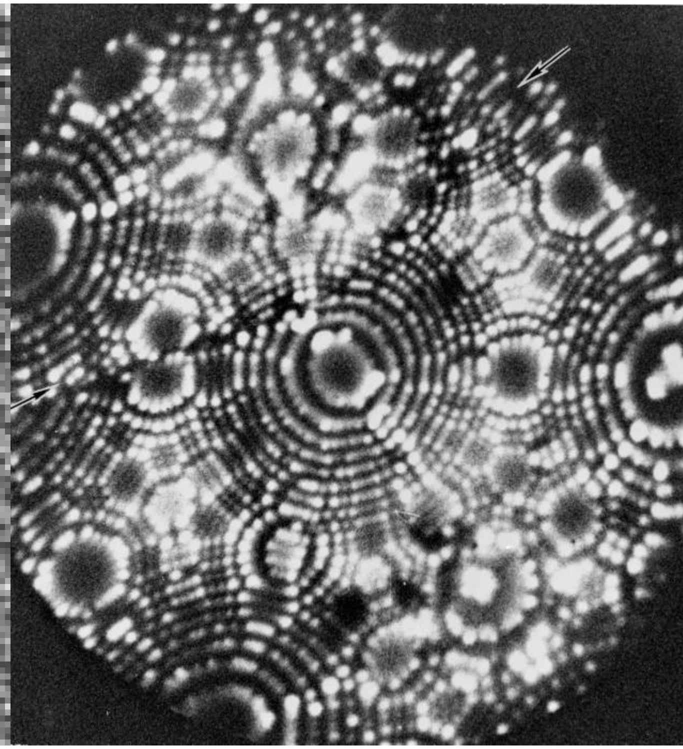


hcp 12

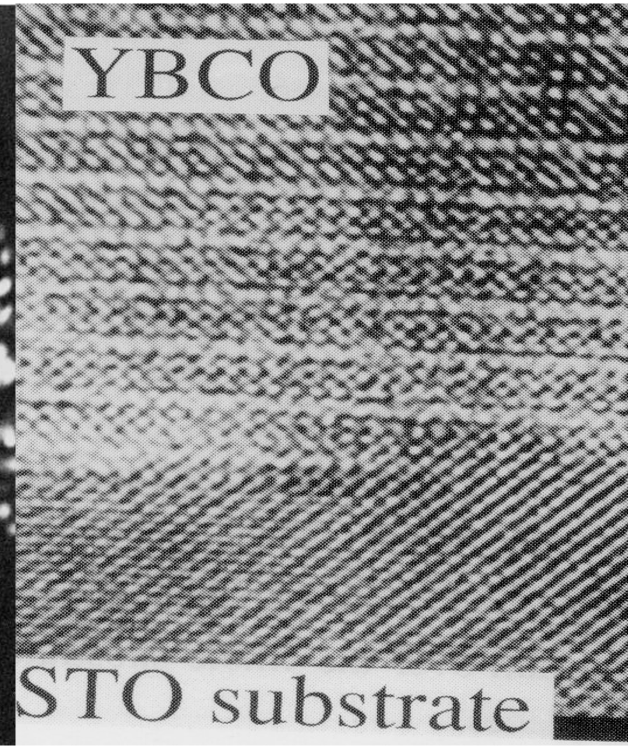
Crystal structure determination



Scanning tunneling microscope



Field ion microscope



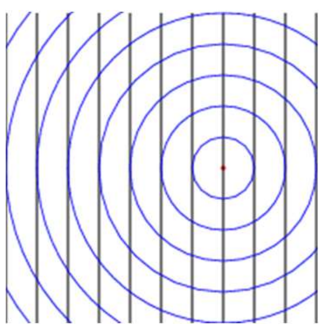
Transmission electron microscope

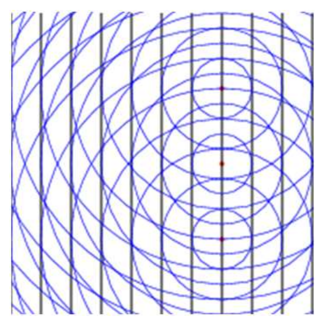
Usually x-ray diffraction is used to determine the crystal structure

Crystal diffraction (Beugung)

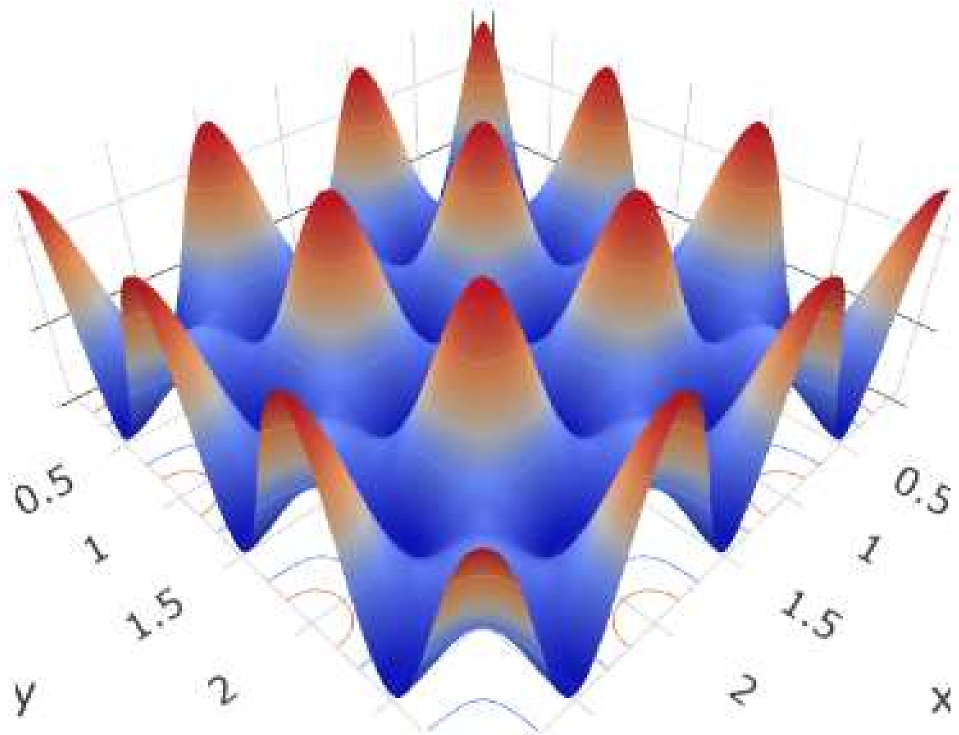
Everything moves like a wave but exchanges energy and momentum as a particle

light	photons
sound	phonons
electron waves	electrons
neutron waves	neutrons
positron waves	positrons
plasma waves	plasmons



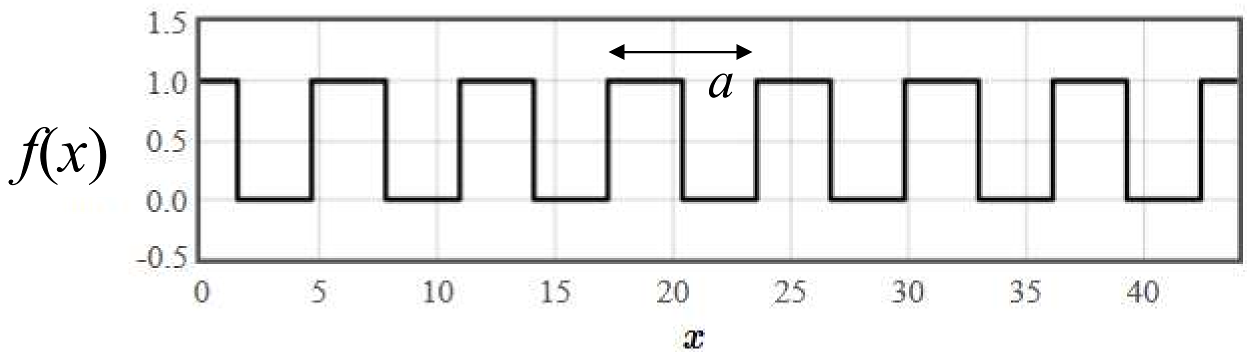


Periodic functions



Use a Fourier series to describe periodic functions

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

multiply by $\cos(2\pi p'x/a)$ and integrate over a period.

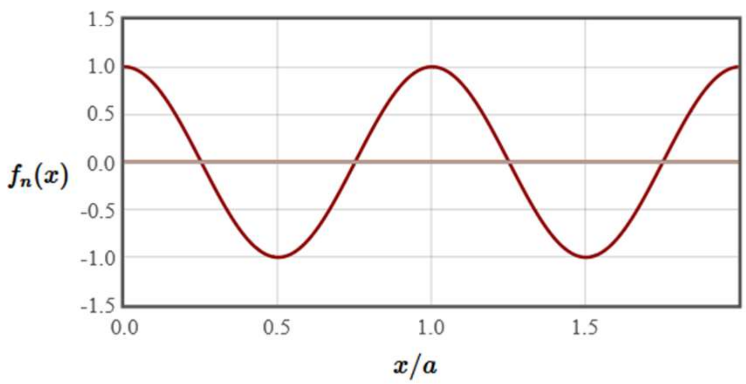
$$\int_0^a f(x)\cos\left(2\pi p'x/a\right)dx = c_p \int_0^a \cos\left(2\pi p'x/a\right)\cos\left(2\pi p'x/a\right)dx = \frac{ac_{p'}}{2}$$

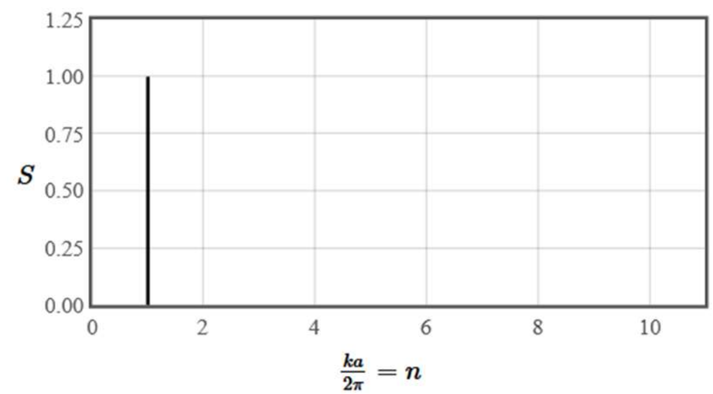
$$c_p = \frac{2}{a}\int_0^a f(x)\cos\left(2\pi px/a\right)dx$$

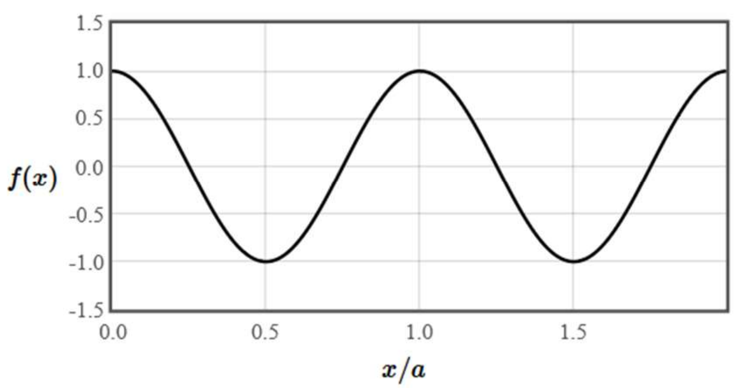
Fourier synthesis

A periodic function with period a can be written as a Fourier series of the form,

$$f(x) = A_0 + \sum_n A_n \left(\cos(\theta_n)\cos(2\pi n x/a) + \sin(\theta_n)\sin(2\pi n x/a)\right).$$





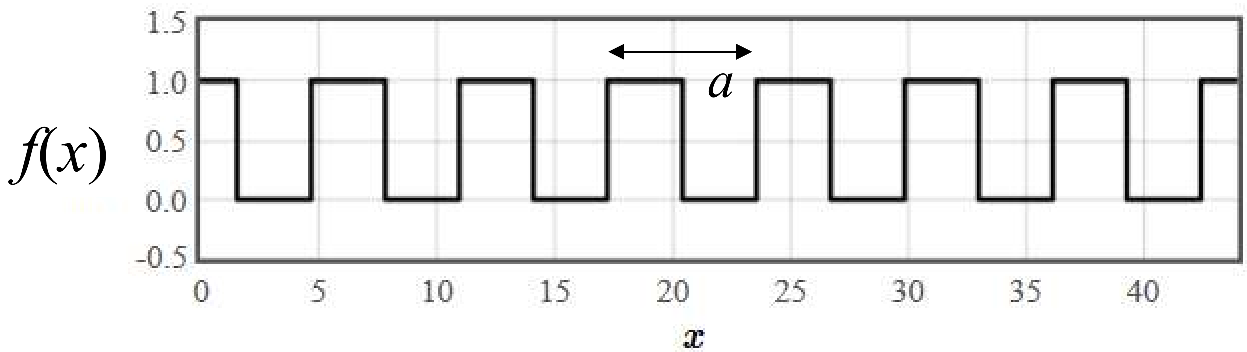


Number of periods displayed: 2

$A_0 = 0$

$A_1 = 1$	$\theta_1 = 0\pi$
$A_2 = 0$	$\theta_2 = 0\pi$
$A_3 = 0$	$\theta_3 = 0\pi$
$A_4 = 0$	$\theta_4 = 0\pi$
$A_5 = 0$	$\theta_5 = 0\pi$
$A_6 = 0$	$\theta_6 = 0\pi$
$A_7 = 0$	$\theta_7 = 0\pi$
$A_8 = 0$	$\theta_8 = 0\pi$
$A_9 = 0$	$\theta_9 = 0\pi$
$A_{10} = 0$	$\theta_{10} = 0\pi$
$A_{11} = 0$	$\theta_{11} = 0\pi$

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

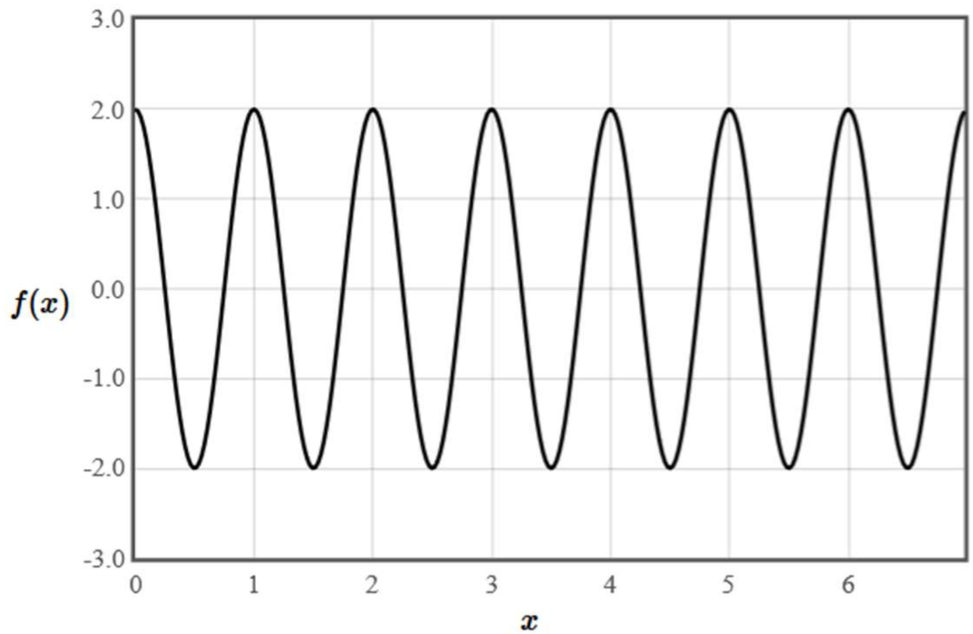
$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$f(x) = \sum_{G=-\infty}^{\infty} f_G e^{iGx} \qquad f_G = \frac{c_p}{2} - i\frac{s_p}{2} \qquad G = \frac{2\pi p}{a}$$

For real functions: $f_G^* = f_{-G}$

reciprocal lattice vector

Fourier series in 1-D



square triangle sawtooth comb

$f_0 = 0$ - +

$f_1 = f^*_{-1} = 1$ - + $+i\ (0)$ - +

$f_2 = f^*_{-2} = 0$ - + $+i\ (0)$ - +

$f_3 = f^*_{-3} = 0$ - + $+i\ (0)$ - +

$f_4 = f^*_{-4} = 0$ - + $+i\ (0)$ - +

$f_5 = f^*_{-5} = 0$ - + $+i\ (0)$ - +

Determine the Fourier coefficients in 1-D

$$f(x) = \sum_G f_G e^{iGx}$$

Multiply by $e^{-iG'x}$ and integrate over a period a

$$\int_{\text{unit cell}} f(x)\, e^{-iG'x} dx = \int_{unit\ cell} \sum_G f_G e^{i(G-G')x} dx \quad = f_{G'} a$$

$$f_G = \frac{1}{a} \int_{-\infty}^{\infty} f_{cell}(x) e^{-iGx} dx$$

The Fourier coefficient is proportional to the Fourier transform of the pattern that gets repeated on the Bravais lattice, evaluated at that G-vector.

Fourier series in 1-D, 2-D, or 3-D

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Reciprocal lattice vectors *G*
(depend on the Bravais lattice)

Structure factors
(complex numbers)

$$\vec{T}_{hkl} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \qquad \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0, & \text{for } i \neq j \end{cases}$$

$$\vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$$

Fourier series in 1-D, 2-D, or 3-D

In two or three dimensions, a periodic function can be thought of as a pattern repeated on a Bravais lattice. It can be written as a Fourier series

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Reciprocal lattice vectors
(depend on the Bravais lattice)

Structure factors
(complex numbers)

In 1-D:

$$\vec{G} = \nu\vec{b} \qquad \nu = -\infty \ldots -1, 0, 1, \ldots \infty \qquad \left|\vec{b}\right| = \frac{2\pi}{a}$$

Reciprocal lattice (Reziprokes Gitter)

Any periodic function can be written as a Fourier series

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Reciprocal lattice vector *G*

Structure factor

$$\vec{G} = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3$$

ν_i integers

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

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

Reciprocal lattice (Reziprokes Gitter)

$$\text{sc:} \qquad \vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\hat{y}, \quad \vec{a}_3 = a\hat{z},$$

$$\vec{b}_1 = \frac{2\pi}{a}\hat{k}_x, \quad \vec{b}_2 = \frac{2\pi}{a}\hat{k}_y, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{k}_z.$$

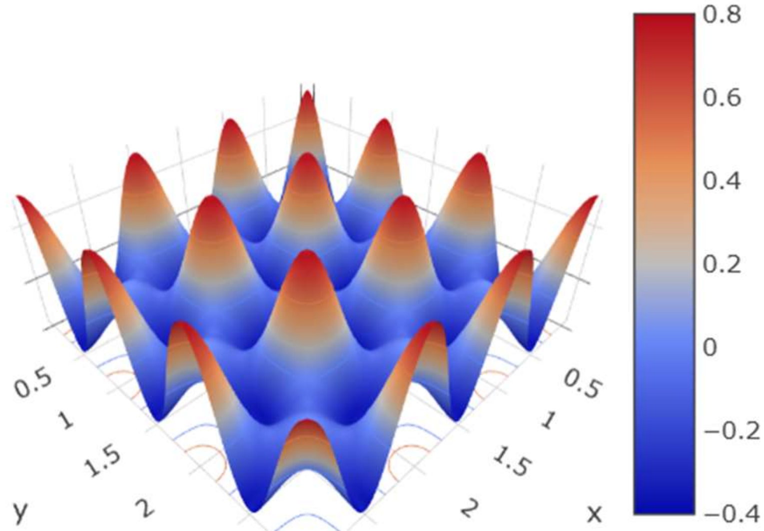
$$\text{fcc:} \qquad \vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{z}), \quad \vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}), \quad \vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z}),$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{k}_x - \hat{k}_y + \hat{k}_z), \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_y - \hat{k}_z), \quad \vec{b}_3 = \frac{2\pi}{a}(-\hat{k}_x + \hat{k}_y + \hat{k}_z).$$

$$\text{bcc:} \qquad \vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}), \quad \vec{a}_2 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}), \quad \vec{a}_3 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z}),$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_y), \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{k}_y + \hat{k}_z), \quad \vec{b}_3 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_z).$$

Two dimensional periodic functions



$f_{00} = 0$ - +

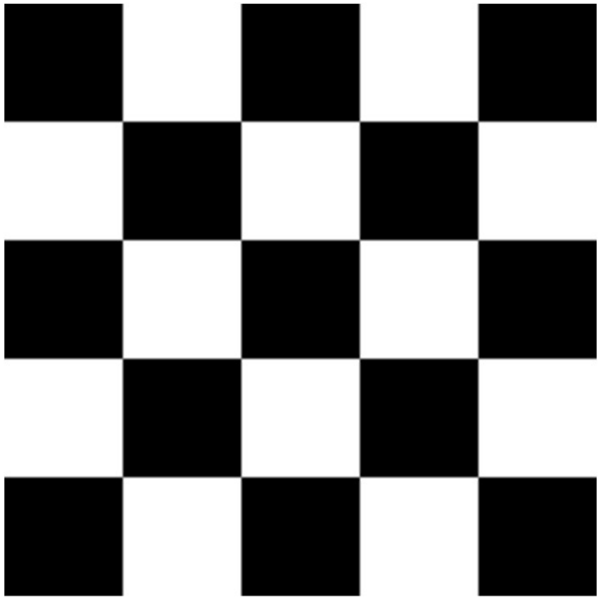
$f_{01} = f^*_{0-1} = 0.1$ - + $+i\ (0)$ - +

$f_{10} = f^*_{-10} = 0.1$ - + $+i\ (0)$ - +

$f_{11} = f^*_{-1-1} = 0.1$ - + $+i\ (0)$ - +

$f_{1-1} = f^*_{-11} = 0.1$ - + $+i\ (0)$ - +

Determine the Fourier coefficients



$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp\left(i\vec{G} \cdot \vec{r}\right)$$

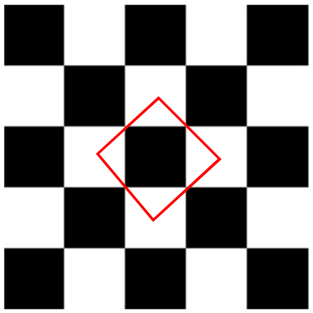
Determine the Fourier coefficients

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp\left(i\vec{G}\cdot\vec{r}\right)$$

Multiply by $\exp(-i\vec{G}'\cdot\vec{r})$ and integrate over a unit cell

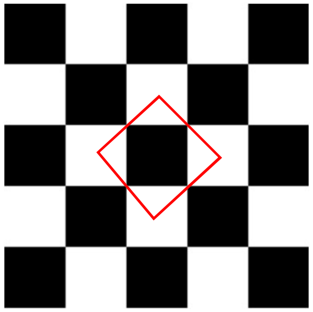
$$\int_{\text{unit cell}} f(\vec{r})\exp(-i\vec{G}'\cdot\vec{r})d\vec{r} = \sum_{\vec{G}} \int_{\text{unit cell}} f_{\vec{G}}\exp(-i\vec{G}'\cdot\vec{r})\exp(i\vec{G}\cdot\vec{r})d\vec{r}$$

$$f_{\vec{G}} = \frac{1}{V_{\text{uc}}} \int_{\text{unit cell}} f(\vec{r})\exp(-i\vec{G}\cdot\vec{r})d\vec{r}$$



Determine the Fourier coefficients

$$f_{\vec{G}} = \frac{C}{a^2} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \exp(-i\vec{G} \cdot \vec{r}) dx dy.$$



$$f_{\vec{G}} = \frac{C}{a^2} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \int_{-\sqrt{2}a/4}^{\sqrt{2}a/4} \exp(-iG_x x) \exp(-iG_y y) dx dy,$$

$$f_{\vec{G}} = \frac{C}{a^2} \frac{\left(\exp(-i\sqrt{2}G_x a/4) - \exp(i\sqrt{2}G_x a/4)\right)\left(\exp(-i\sqrt{2}G_y a/4) - \exp(i\sqrt{2}G_y a/4)\right)}{-G_x G_y}.$$

$$f_{\vec{G}} = \frac{4C}{a^2} \frac{\sin(\sqrt{2}G_x a/4) \sin(\sqrt{2}G_y a/4)}{G_x G_y}.$$

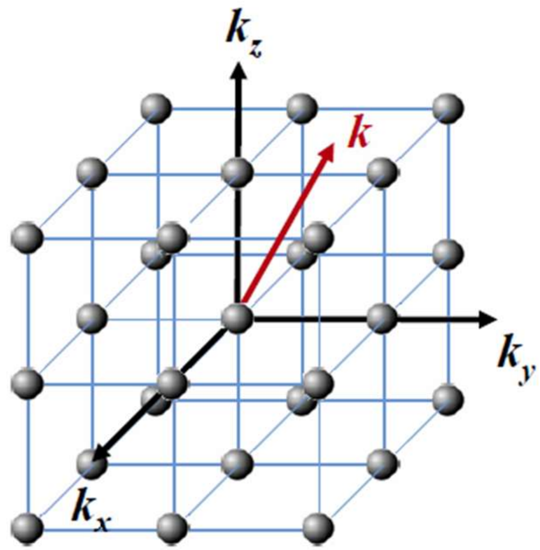
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

k-space is the space of all wave-vectors.

A *k*-vector points in the direction a wave is propagating.

wavelength: $\lambda = \frac{2\pi}{|\vec{k}|}$

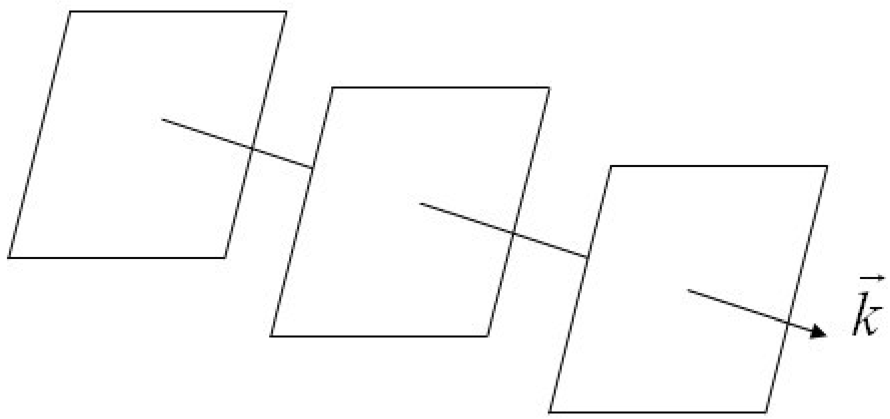
momentum: $\vec{p} = \hbar\vec{k}$



Plane waves (Ebene Wellen)

$$e^{i\vec{k}\cdot\vec{r}} = \cos\left(\vec{k}\cdot\vec{r}\right) + i\sin\left(\vec{k}\cdot\vec{r}\right)$$

$$\lambda = \frac{2\pi}{\left|\vec{k}\right|}$$



$$\exp\left(i\vec{k}\cdot\left(\vec{r}+\vec{r}_{\perp}\right)\right) = \exp\left(i\vec{k}\cdot\vec{r}\right)$$

Most functions can be expressed in terms of plane waves

$$f(\vec{r}) = \int F\left(\vec{k}\right) e^{i\vec{k}\cdot\vec{r}}\, d\vec{k}$$

A *k*-vector points in the direction a wave is propagating.