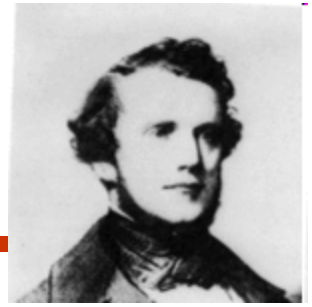
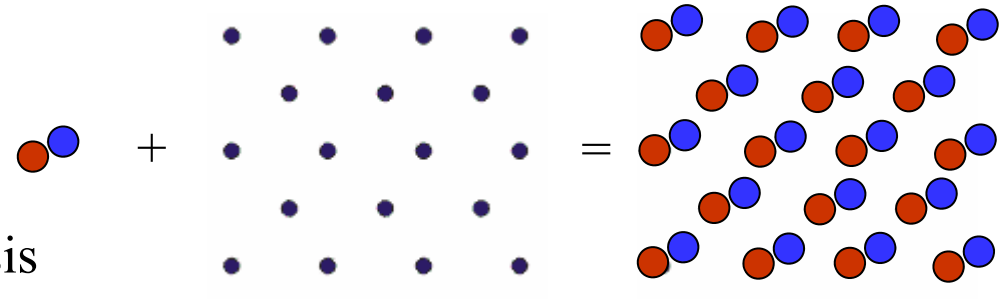
7. Crystal structure, Diffraction

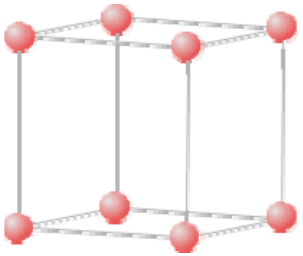
April 10, 2018

Bravais lattice

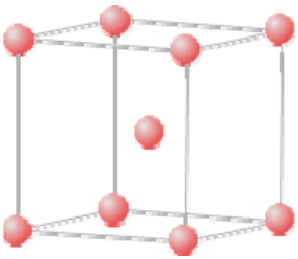


Auguste Bravais

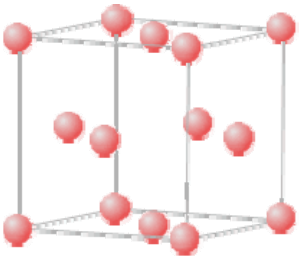




simple cubic



body centered cubic, bcc

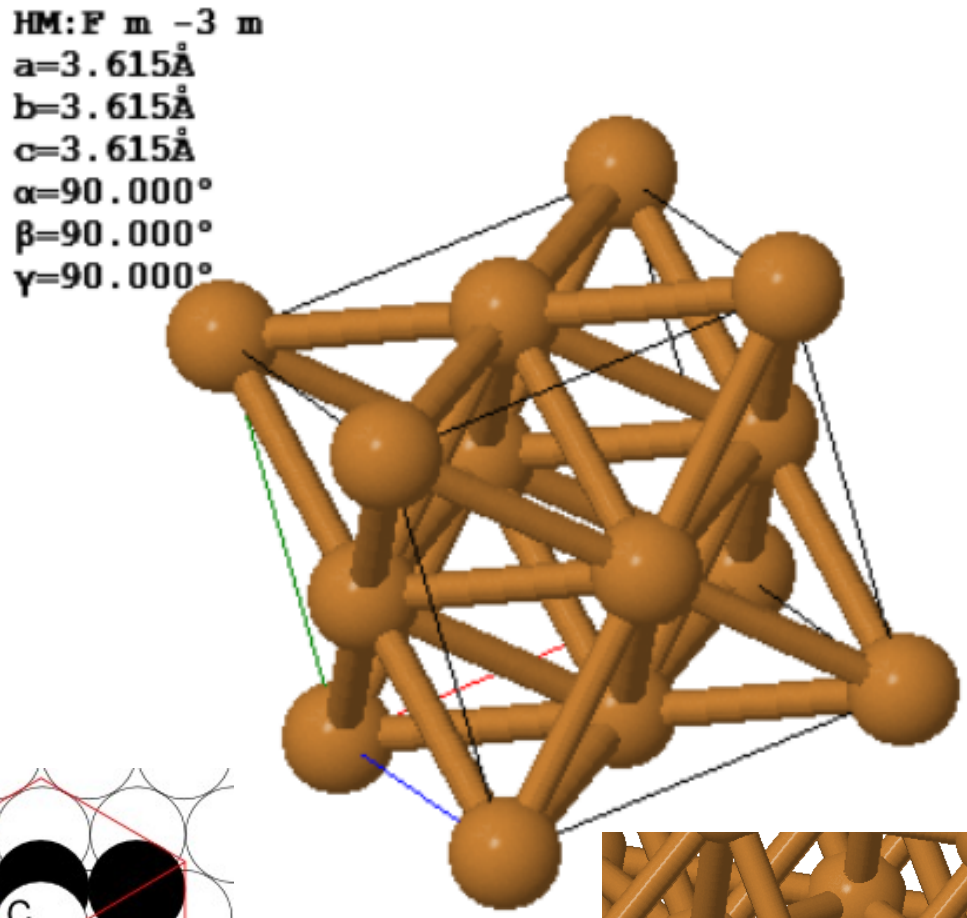


face centered cubic, fcc

fcc

Number 225

Al, Cu,
Ni, Sr,
Rh, Pd,
Ag, Ce,
Tb, Ir,
Pt, Au,
Pb, Th



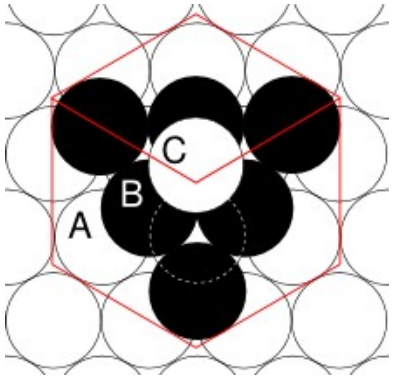
[111]

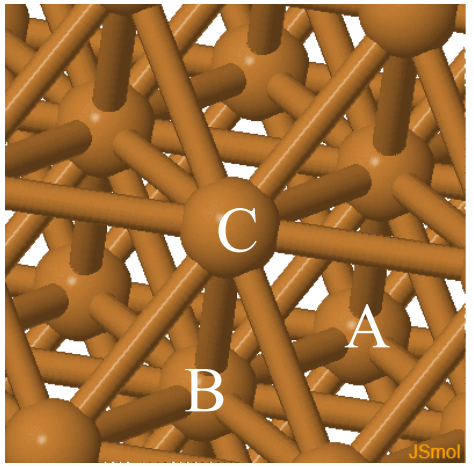
Primitive Vectors:

$$\vec{a}_1 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$



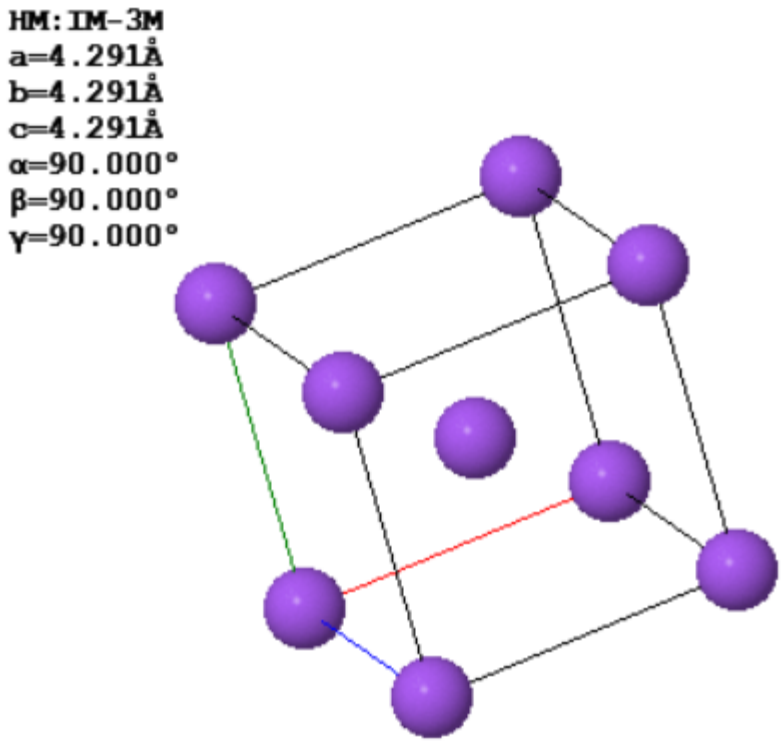


Basis Vector: $\vec{B}_1 = (0,0,0)$

bcc

W
Na
K
V
Cr
Fe
Rb
Nb
Mo
Cs
Ba
Eu
Ta

Number 229



Primitive Vectors:

$$\vec{a}_1 = -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_2 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z}$$

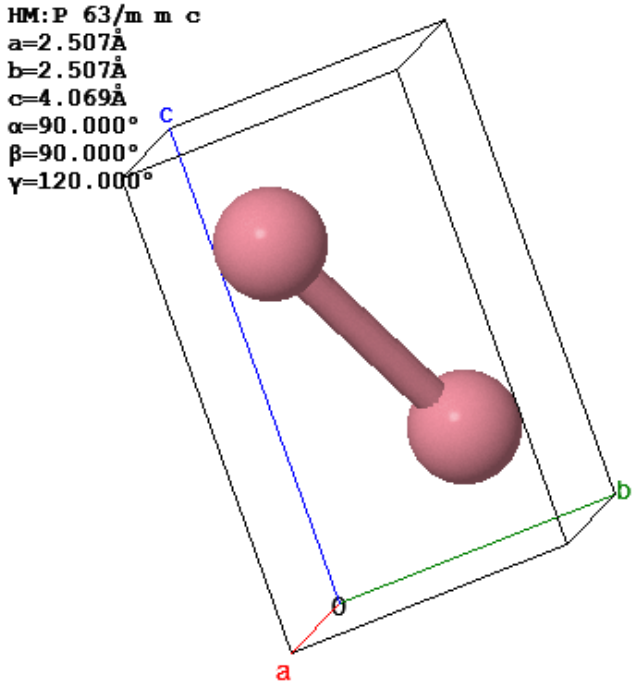
Basis Vector: $\vec{B}_1 = (0,0,0)$

hcp

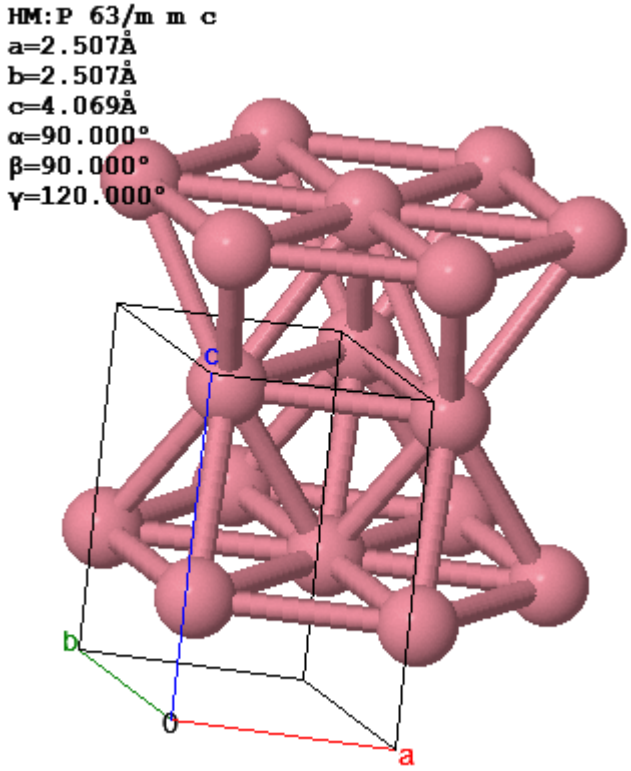
Space group 194

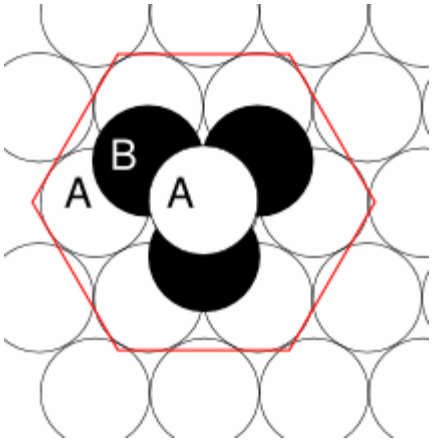
Mg, Be,
Sc, Ti,
Co, Zn,
Y, Zr, Tc,
Ru, Cd,
Gd, Tb,
Dy, Ho,
Er, Tm,
Lu, Hf,
Re, Os,
Tl

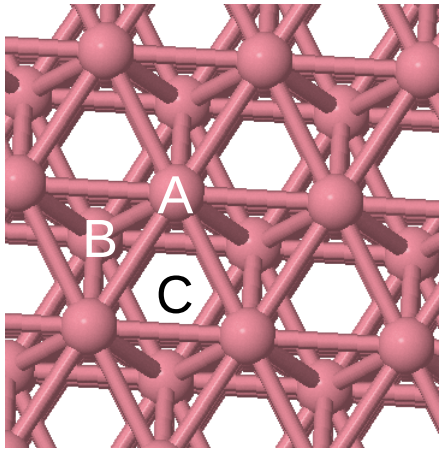
Crystallographic unit cell



Hexagonal unit cell







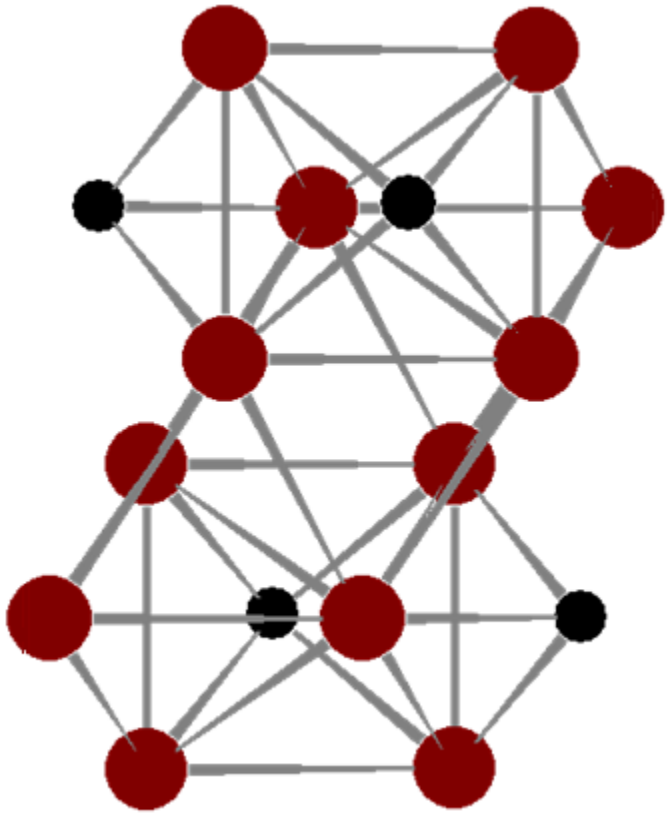
Hexagonal Bravais lattice
Basis vectors:

$$\vec{B}_1 = (0,0,0) \quad \vec{B}_2 = (\tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{2})$$

Asymmetric unit

cell 5.09000 6.74800 4.52300 90.000 90.000 90.000
natom 3
Fe1 26 0.18600 0.06300 0.32800
Fe2 26 0.03600 0.25000 0.85200
C 6 0.89000 0.25000 0.45000
rgnr 62
Cohenite (Cementite) Fe3 C

Unit cell

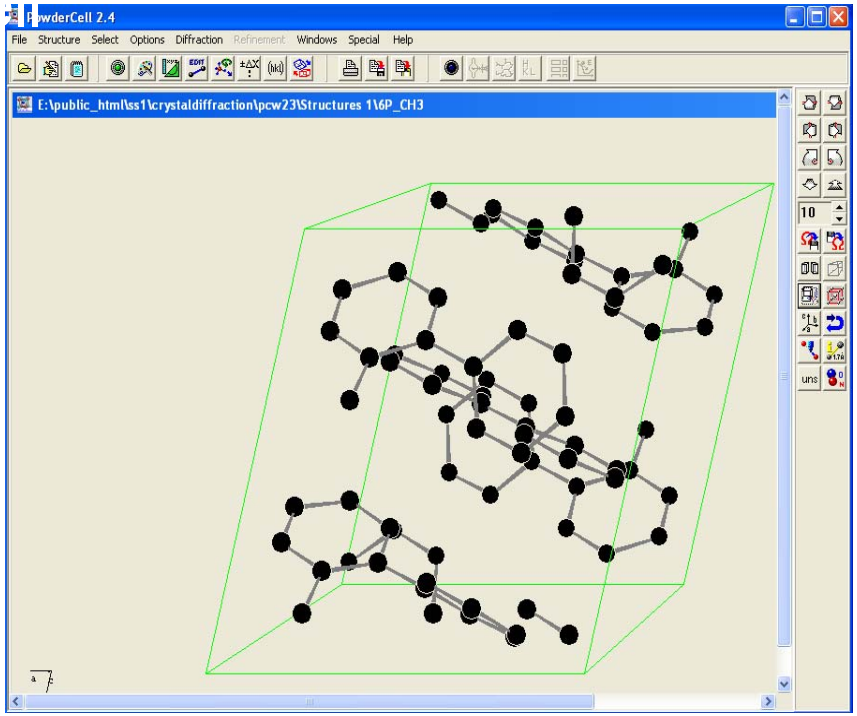


Asymmetric unit

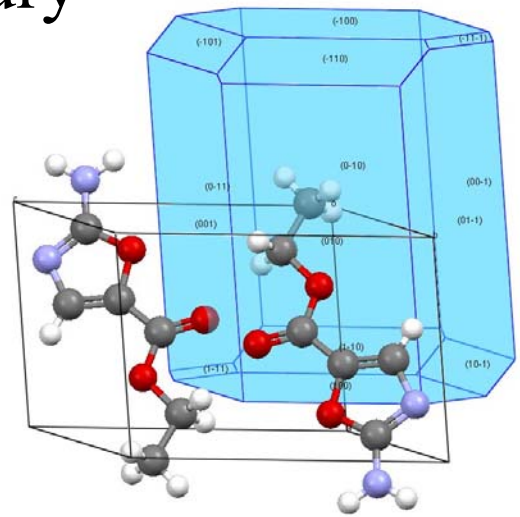
Generated by PowderCell

BAM
Bundesanstalt für Materialforschung und -prüfung

PowderCell



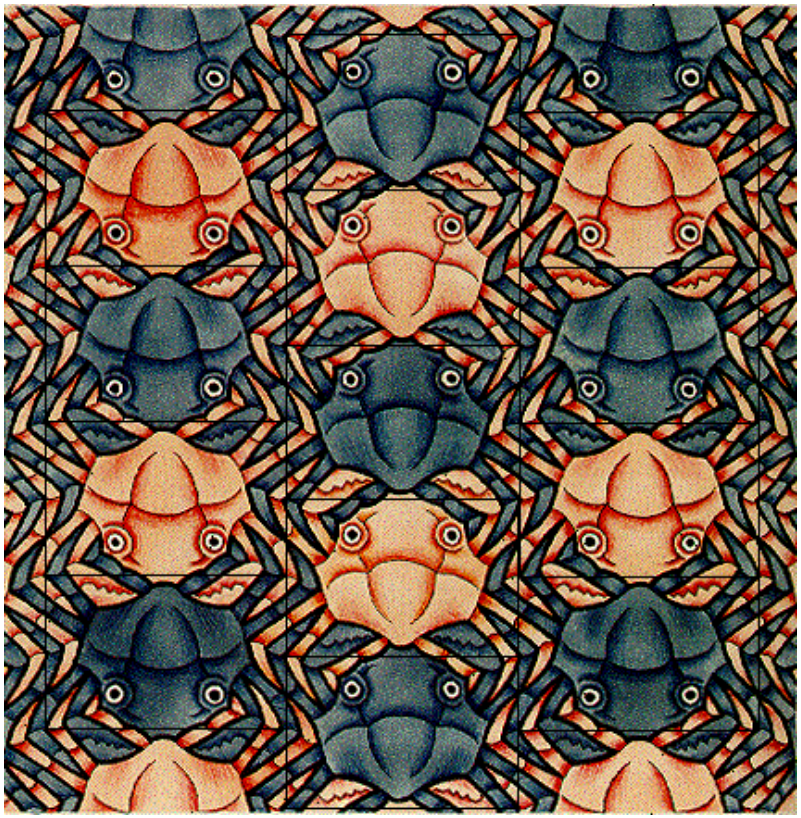
Mercury



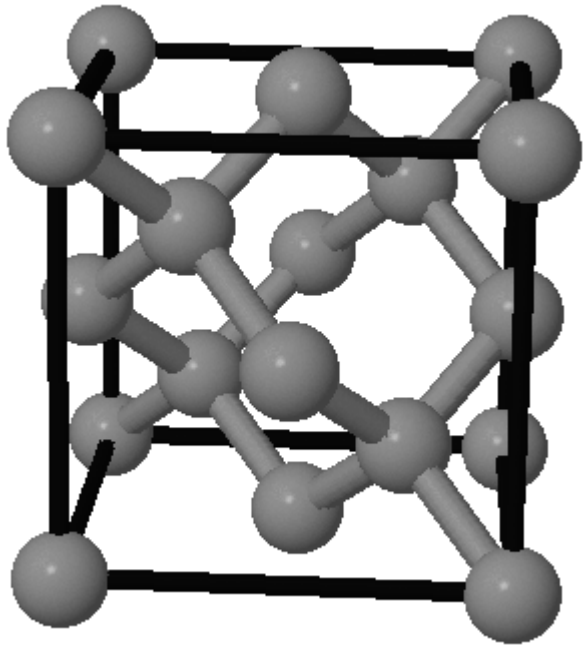
Standard data file: *.cif

http://www.bam.de/de/service/publikationen/powder_cell.htm
https://www.ccdc.cam.ac.uk/Community/csd-community/freemercury/

Inequivalent atoms in the unit cell

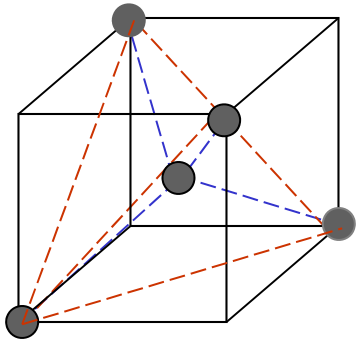


An element can have two distinct positions

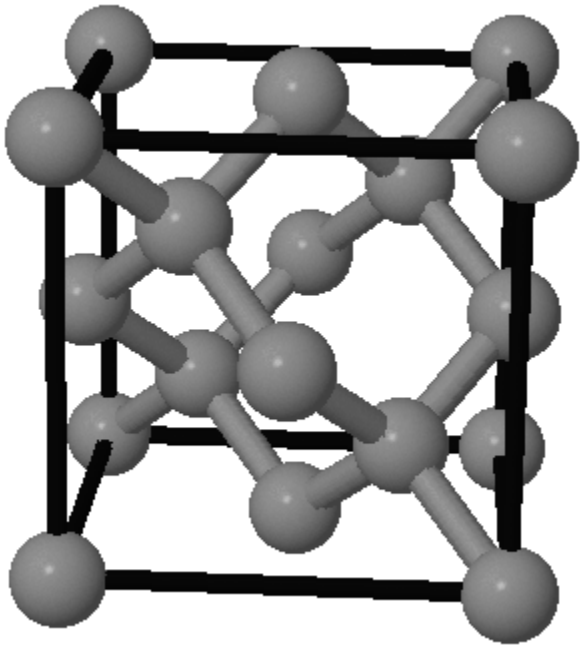


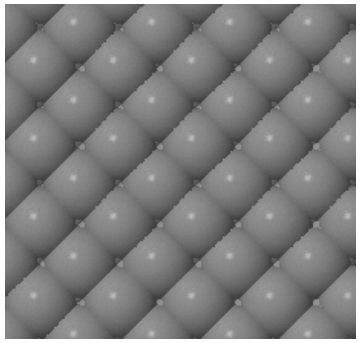
Diamond conventional unit cell

Diamond

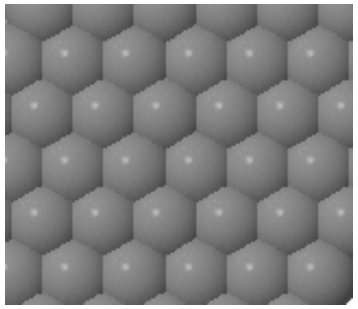


$$a = b = c, \quad \alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$$





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



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

Space group: 227
point group: m3m

Primitive lattice vectors:

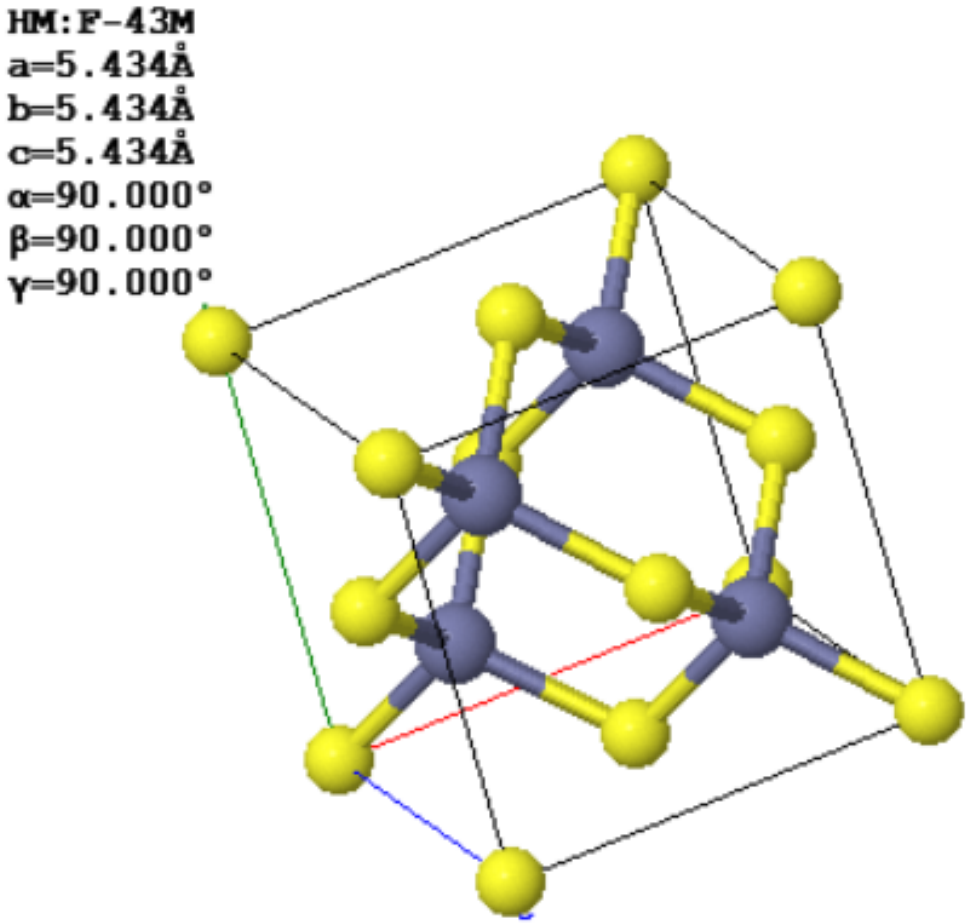
$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}, \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}, \qquad \vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}.$$

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

zincblende

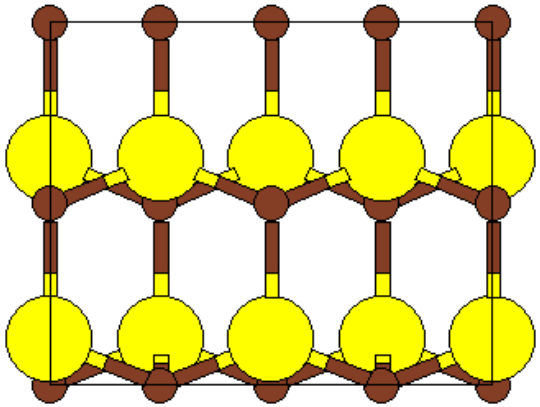
ZnS
GaAs
InP

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



wurtzite

ZnS
ZnO
CdS
CdSe
GaN
AlN

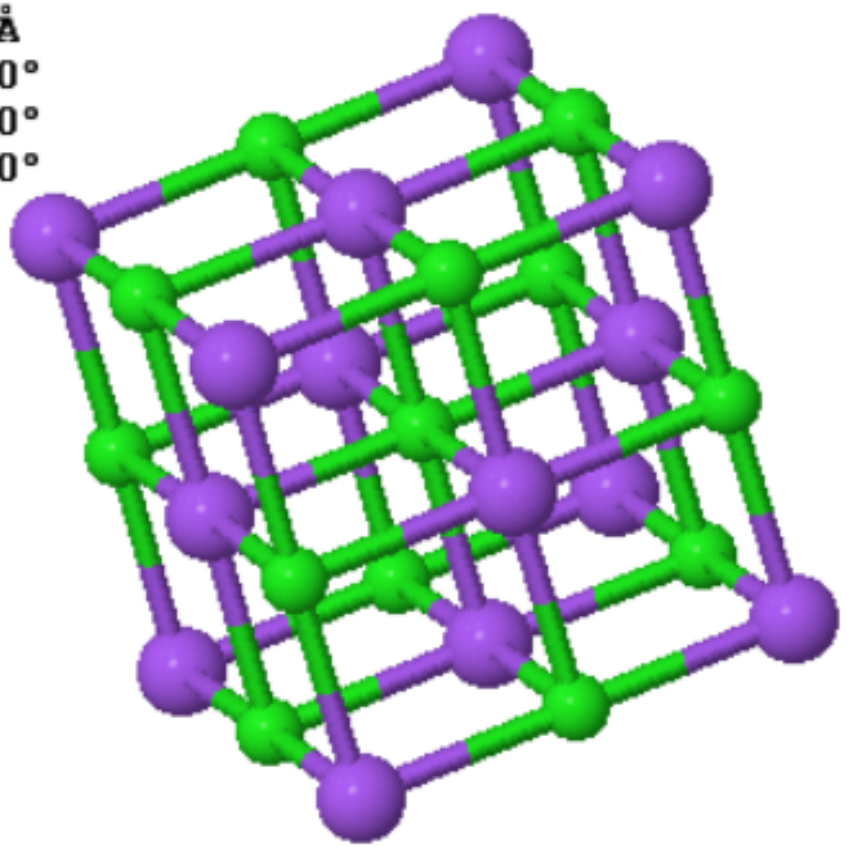


Number 186

There are 2 polytypes of ZnS: zincblende and wurtzite

NaCl

HM:F m -3 m
a=5.639Å
b=5.639Å
c=5.639Å
α=90.000°
β=90.000°
γ=90.000°

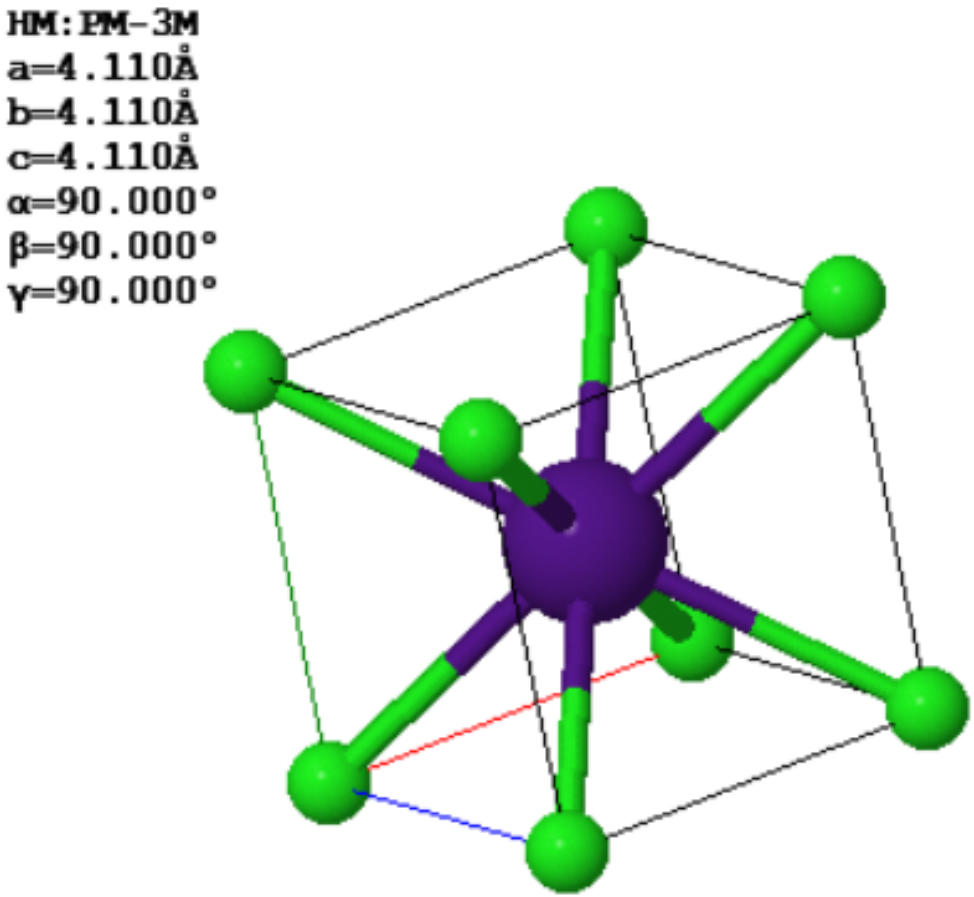


Number 225

Bravais: fcc

CsCl

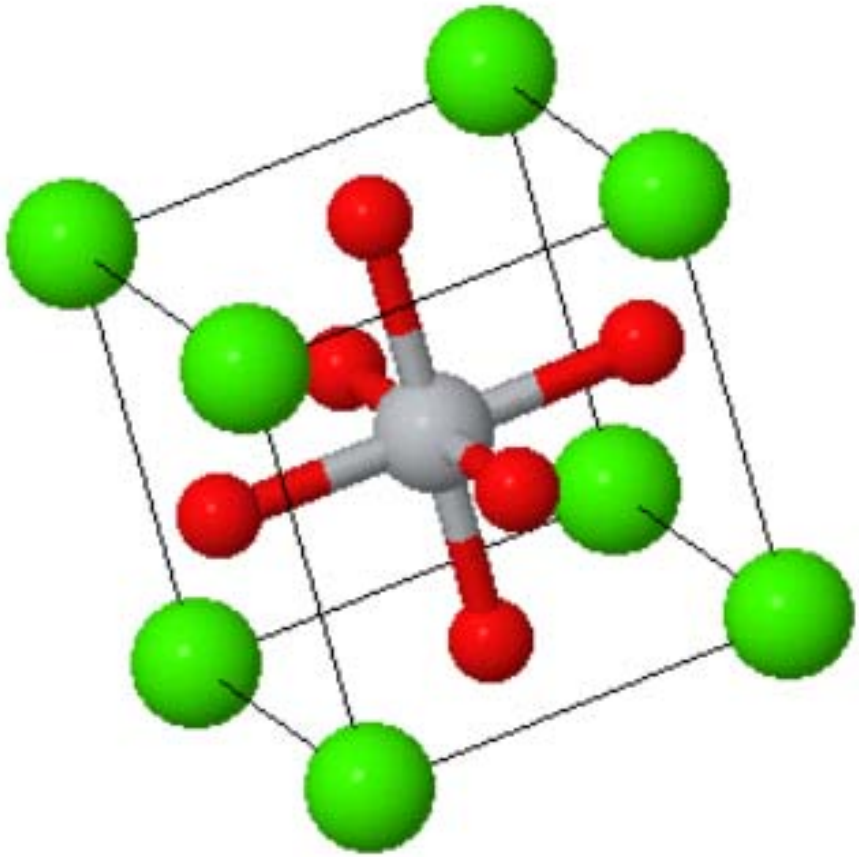
Number 221



perovskite

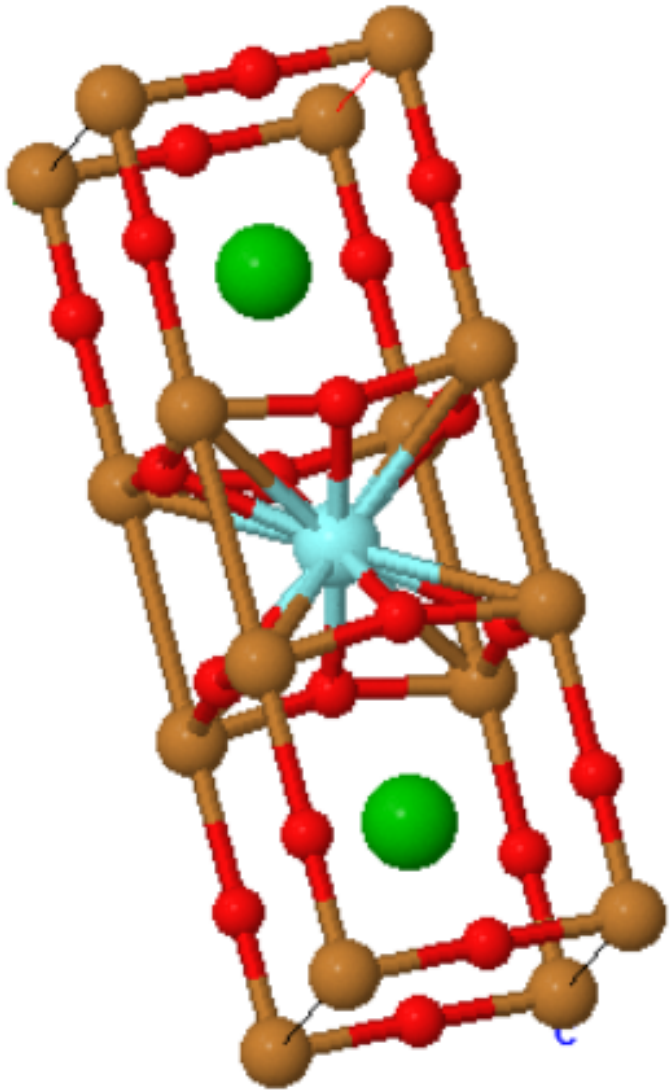
$SrTiO_3$
$LiNbO_3$
$BaTiO_3$
$Pb_xZr_{1-x}TiO_3$

Number 221
simple cubic



$YBa_2Cu_3O_7$

HM:P m m m
a=3.820Å
b=3.885Å
c=11.683Å
α=90.000°
β=90.000°
γ=90.000°

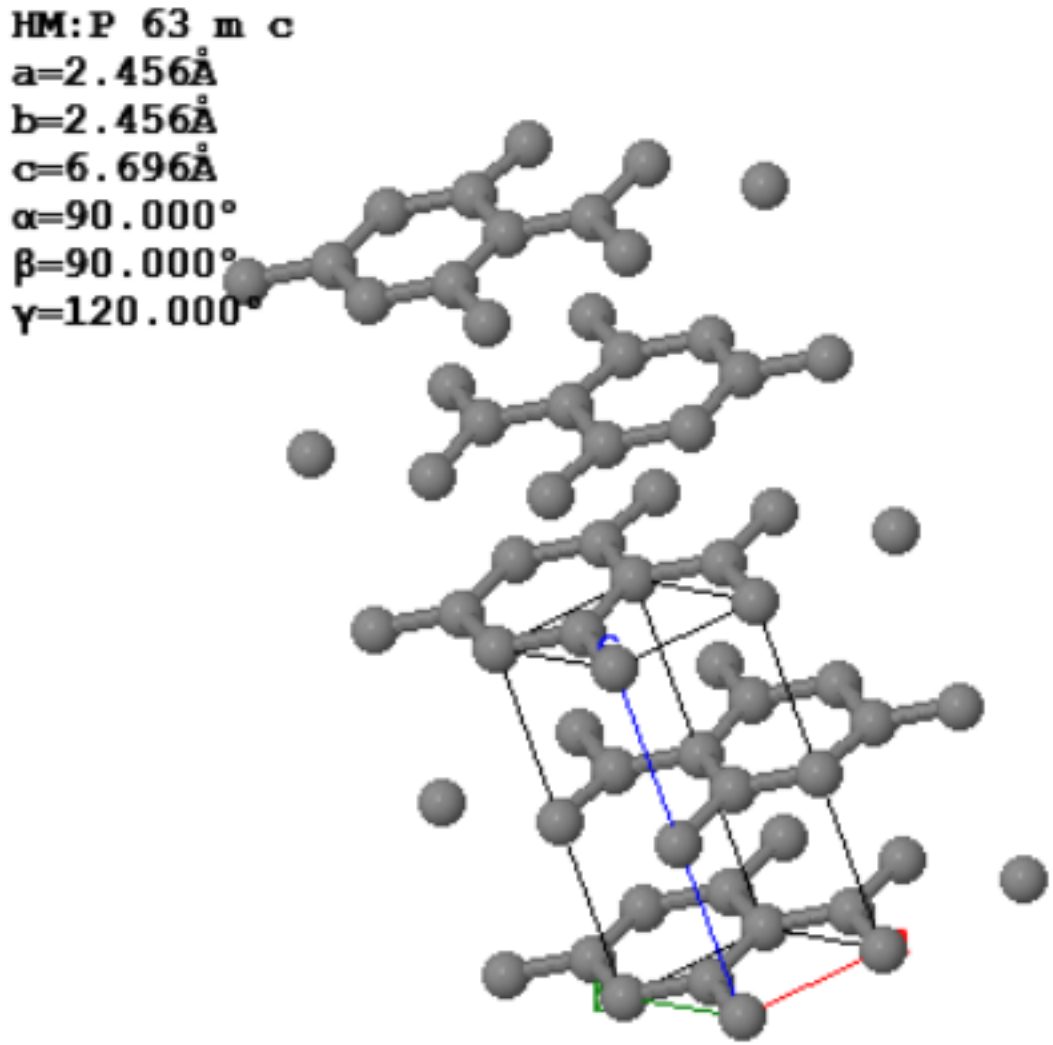


Number 47

graphite

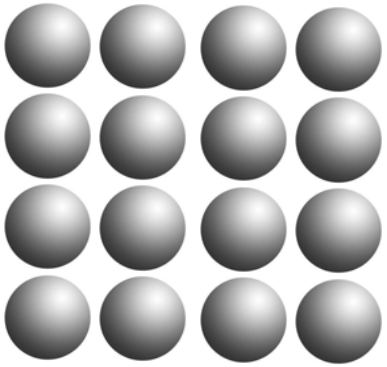
Space group 194

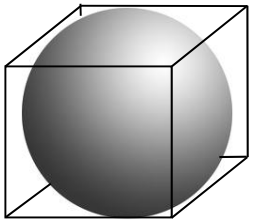
4 inequivalent C atoms in the primitive unit cell



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

atomic packing density



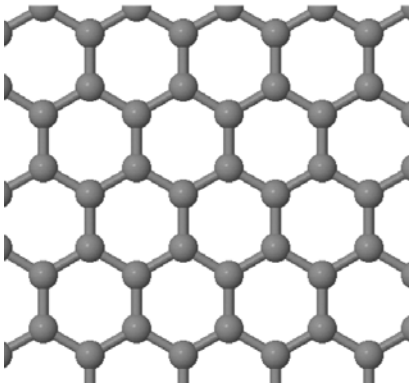


$$\frac{\frac{4}{3}\pi\left(L/2\right)^3}{L^3} = \frac{\pi}{6} \approx 0.52$$

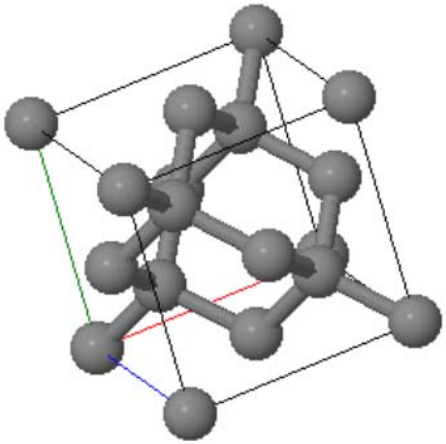
fcc, hcp = 0.74
random close pack = 0.64
simple cubic = 0.52
diamond = 0.34

Coordination number

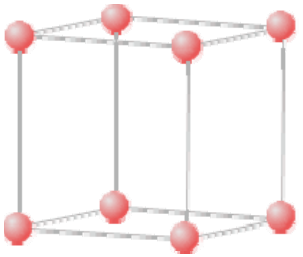
Number of nearest neighbors an atom has in a crystal



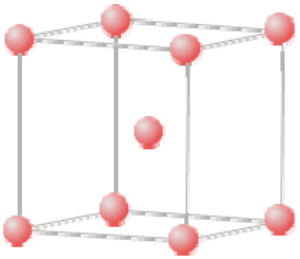
Graphene 3



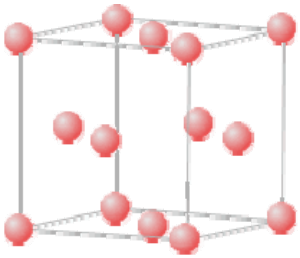
diamond 4



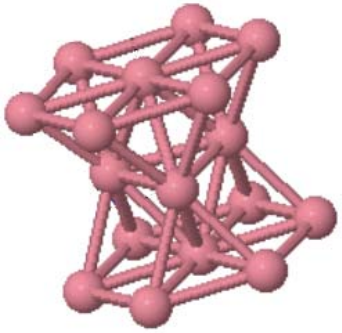
sc 6



bcc 8



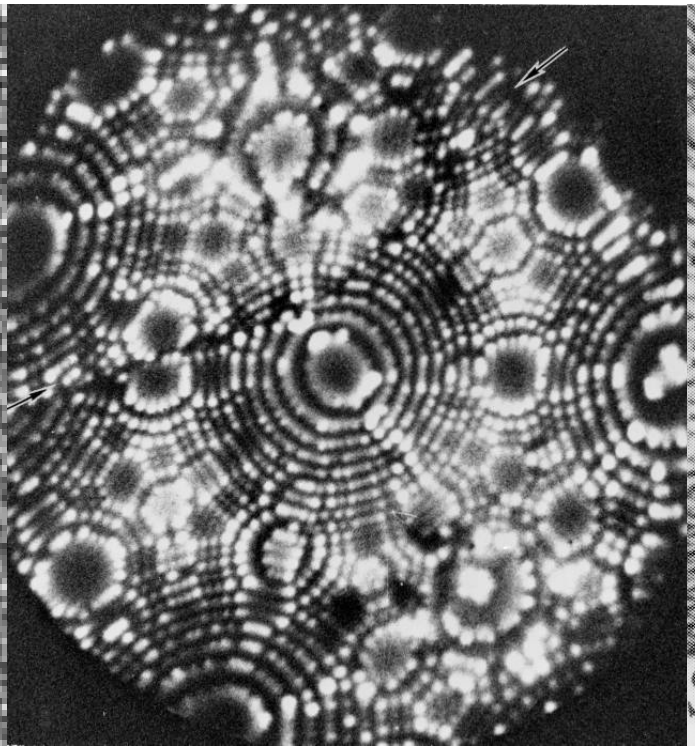
fcc 12



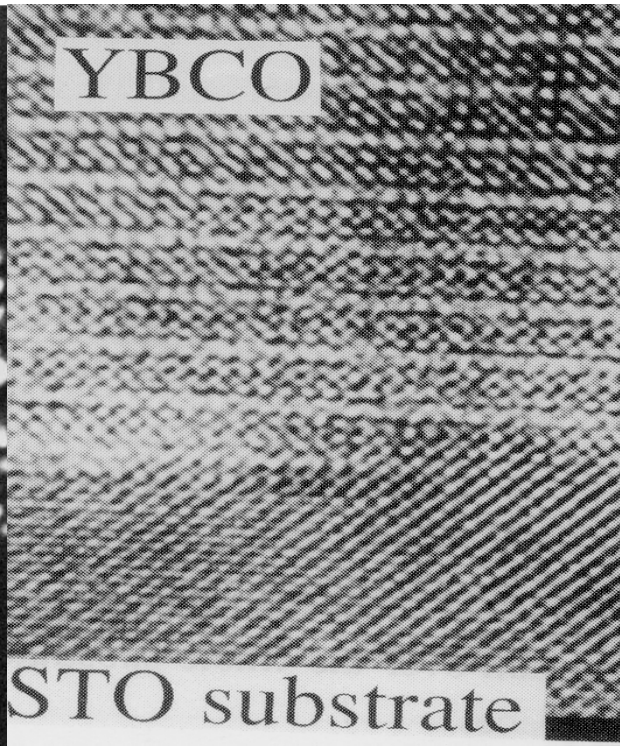
hcp 12

Crystal structure determination

Scanning tunneling microscope



Field ion microscope



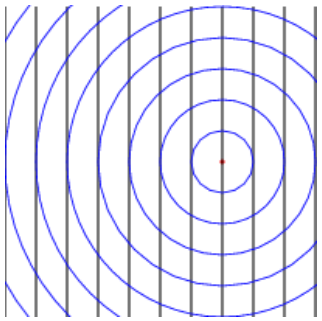
Transmission electron microscope

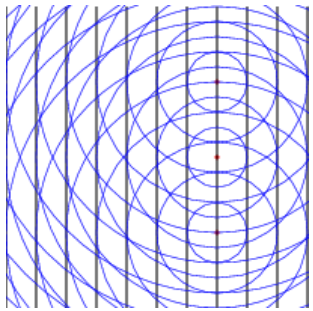
Usually x-ray diffraction is used to determine the crystal structure

Crystal diffraction (Beugung)

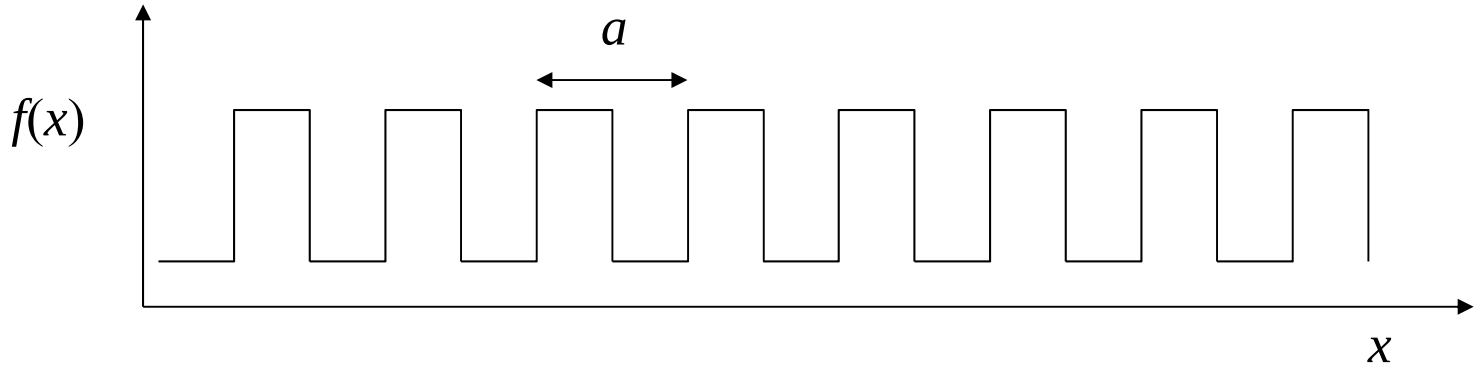
Everything moves like a wave but exchanges energy and momentum as a particle

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





Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

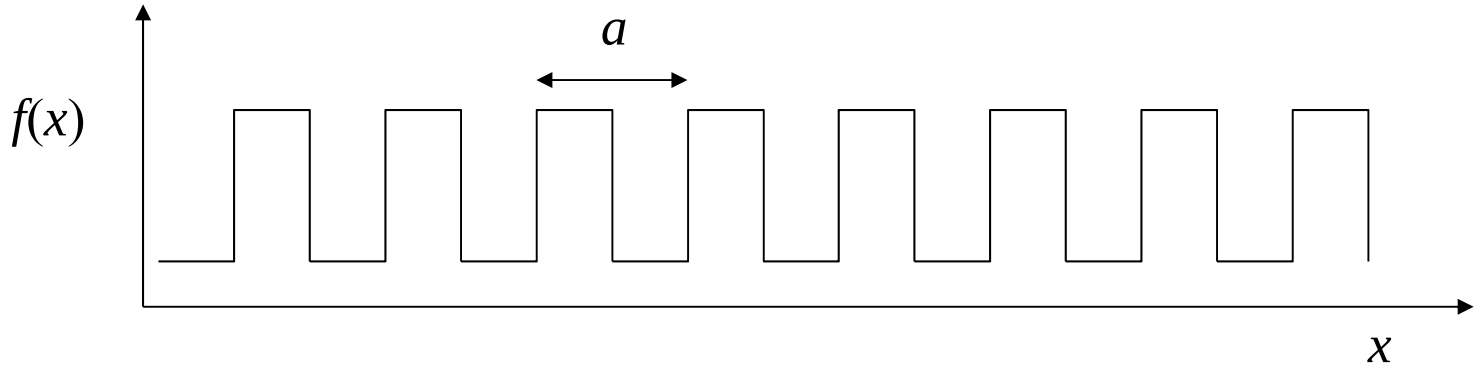
$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

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

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

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

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, 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:

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

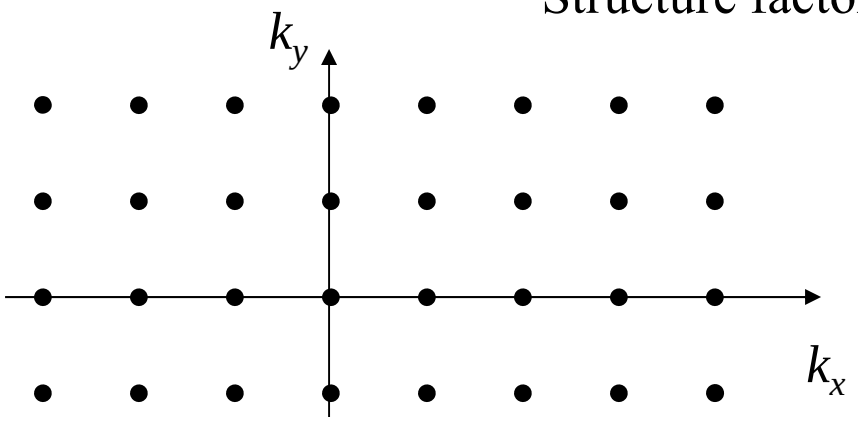
Reciprocal lattice (Reziprokes Gitter)

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



$$\vec{G} = \upsilon_1\vec{b}_1 + \upsilon_2\vec{b}_2 + \upsilon_3\vec{b}_3$$

ν_i integers

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

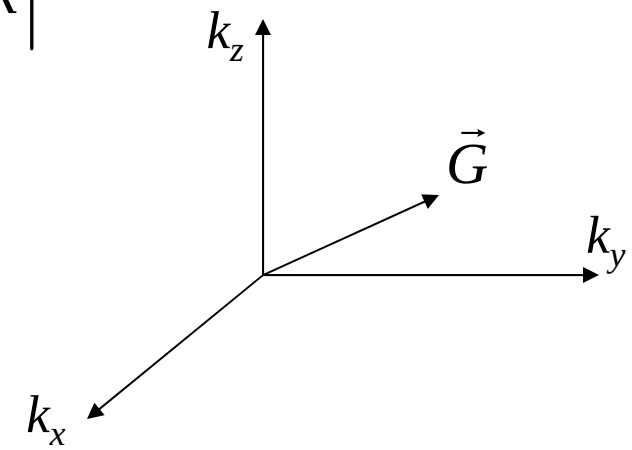
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

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 wave:

$$\exp(i\vec{G}\cdot\vec{r}) = \cos(G_x x + G_y y + G_z z) + i\sin(G_x x + G_y y + G_z z)$$