Course plan

Recap from last week (crystal structure)

Graphene – 2010 Nobel Prize

→ Crystal structures, Lattice vectors, crystal basis etc.

New Goal: Resolve crystal structure of a new 200 K superconductor!

→ Reciprocal space, reciprocal lattice vectors & units, Brillouin zones
→ Scattering theory

Experiments
Scattering triangle
Scattering probability
Bragg's law
Form factor
Structure factor

→ How to resolve crystal structures from scattering experiments

TASKS FOR NEXT WEEK

8 NOBEL PRICES ON SUPERCONDUCTIVITY AND SUPERFLUIDITY

In 1913, Heike Kamerlingh Onnes received the Nobel Prize in Physics "for his investigations on the properties of matter at low temperatures, which led, inter alia, to the production of liquid He4", and the discovery of superconductivity.

In 1962, Lev Davidovich Landau received the Nobel Prize in Physics "for his pioneering theories for condensed matter, specially liquid helium."

In 1972, John Bardeen, Leon N. Cooper and J. Robert Schrieffer received the Nobel Prize in Physics "for the jointly developed theory of superconductivity, usually called the BCS theory."

In 1973, Brian David Josephson received one half of the Nobel Prize in Physics "for his theoretical predictions of the properties of a supercurrent through a tunnel barrier, in particular those phenomena which are generally known as the Josephson Effects.

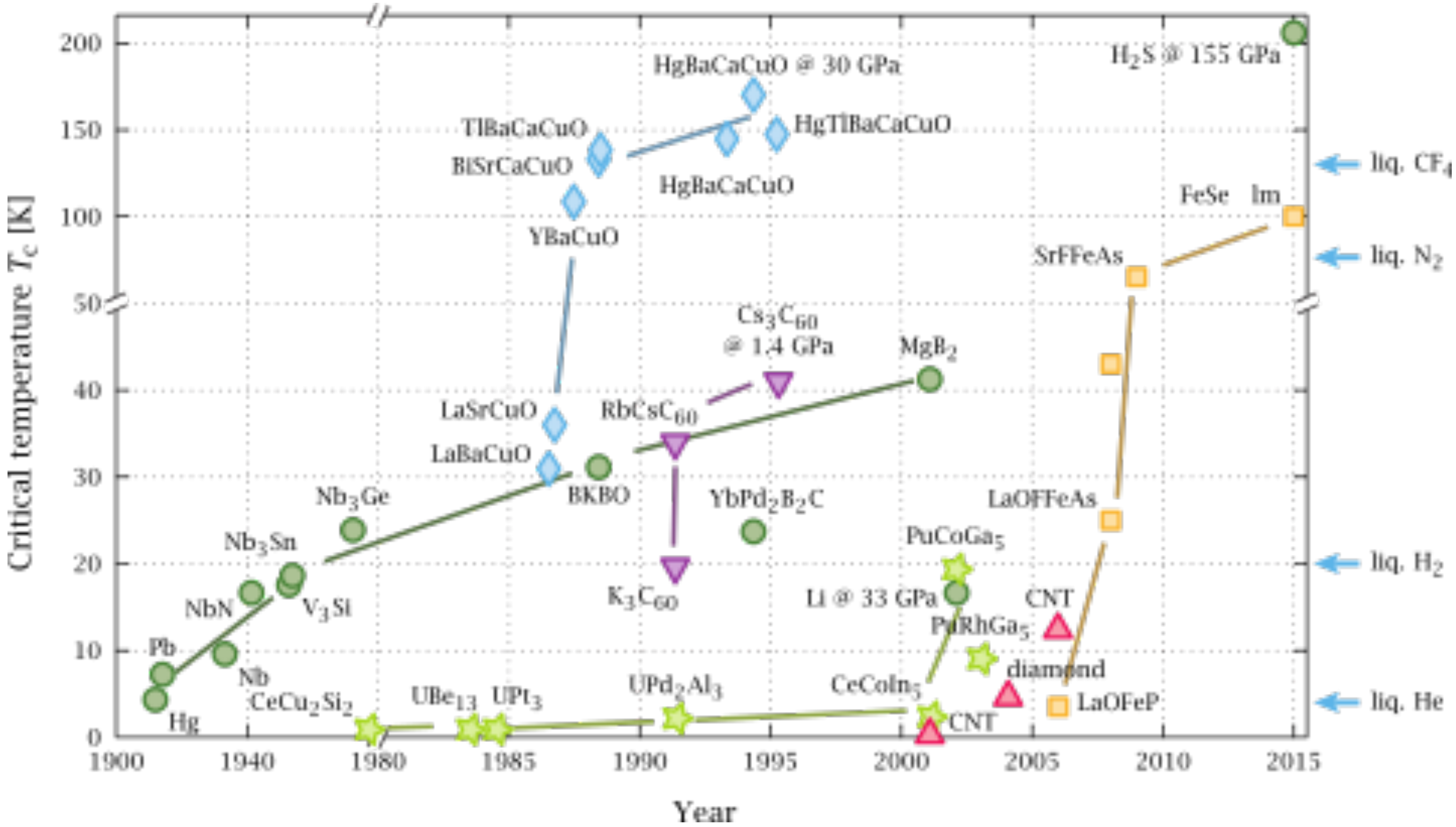
In 1978, Pyotr Leonidovich Kapitsa received one half of the Nobel Prize in Physics "for his basic inventions and discoveries in the area of low temperature physics," which included the discovery of superfluidity in He.

In 1987, J. Georg Bednorz and K. Alexander Müller received the Nobel Prize in Physics "for their important breakthrough in the discovery of superconductivity in ceramic materials."

In 1996, David M. Lee, Douglas D. Osheroff and Robert C. Richardson received the Nobel Prize in Physics "for their discovery of superfluidity in helium-3."

In 2003, Alexei A. Abrikosov, Vitaly L. Ginsburg and Anthony J. Leggett received the Nobel Prize in Physics "for pioneering contributions to the theory of superconductors and superfluids.

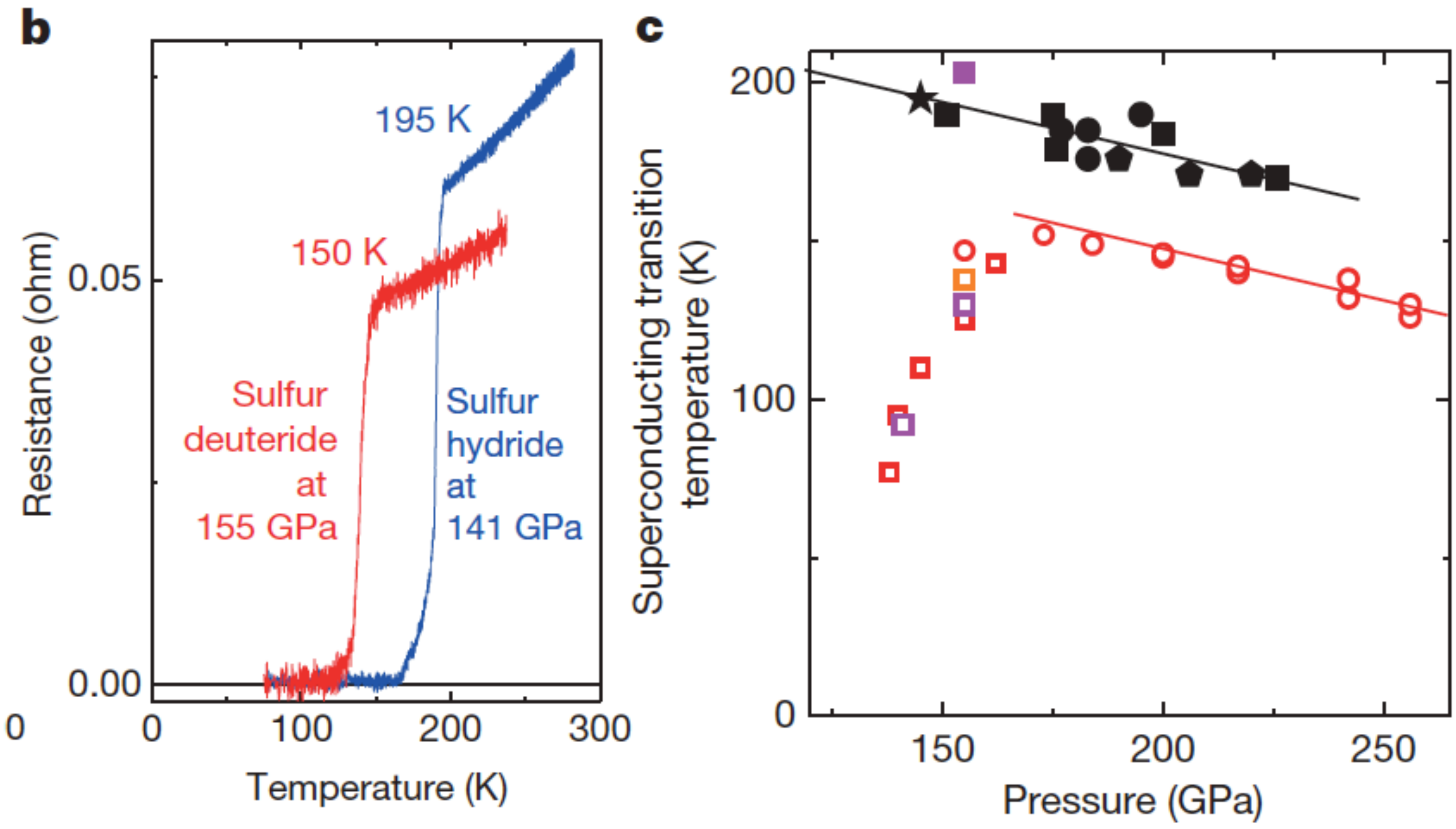
History of superconductivity



https://en.wikipedia.org/wiki/History_of_superconductivity

Hydrogen Sulfide - Cave diving

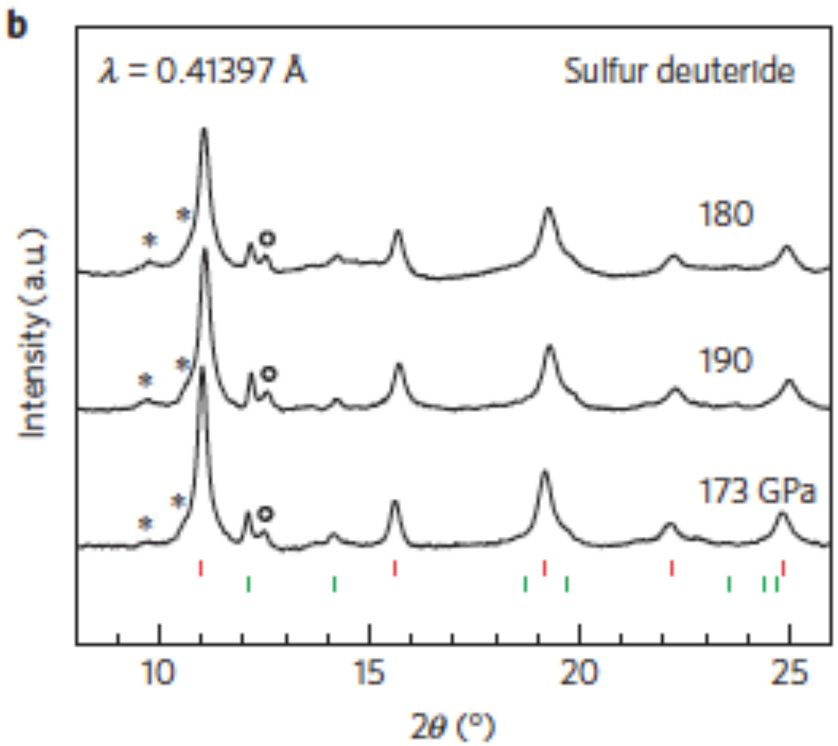
H_2S under pressure - A 200 K superconductor



Nature **525**, 73–76 (03 September 2015)

What crystal structure?

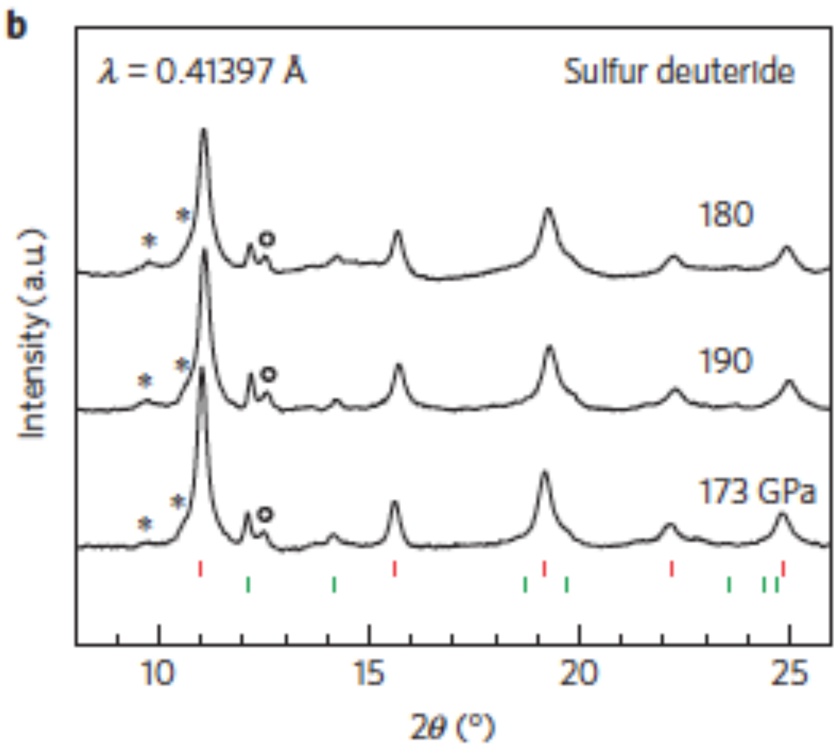
200 K superconductor



Nature Physics 12, 835–838 (2016)

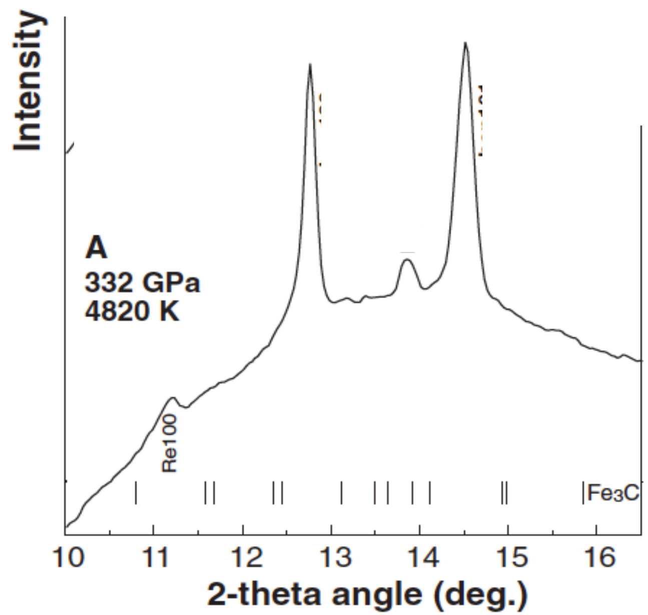
What crystal structure?

200 K superconductor

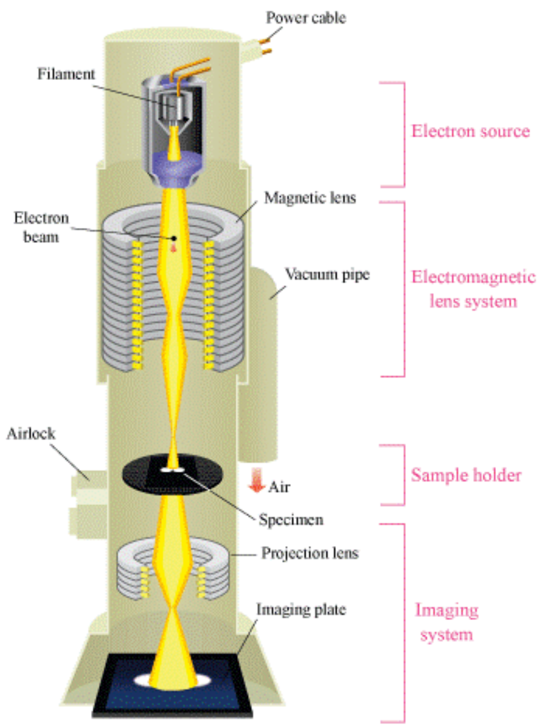


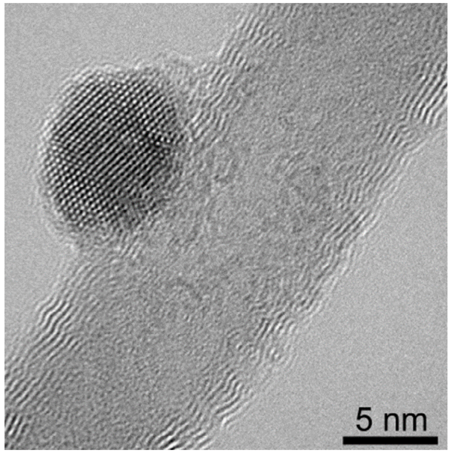
Nature Physics 12, 835–838 (2016)

Iron under pressure



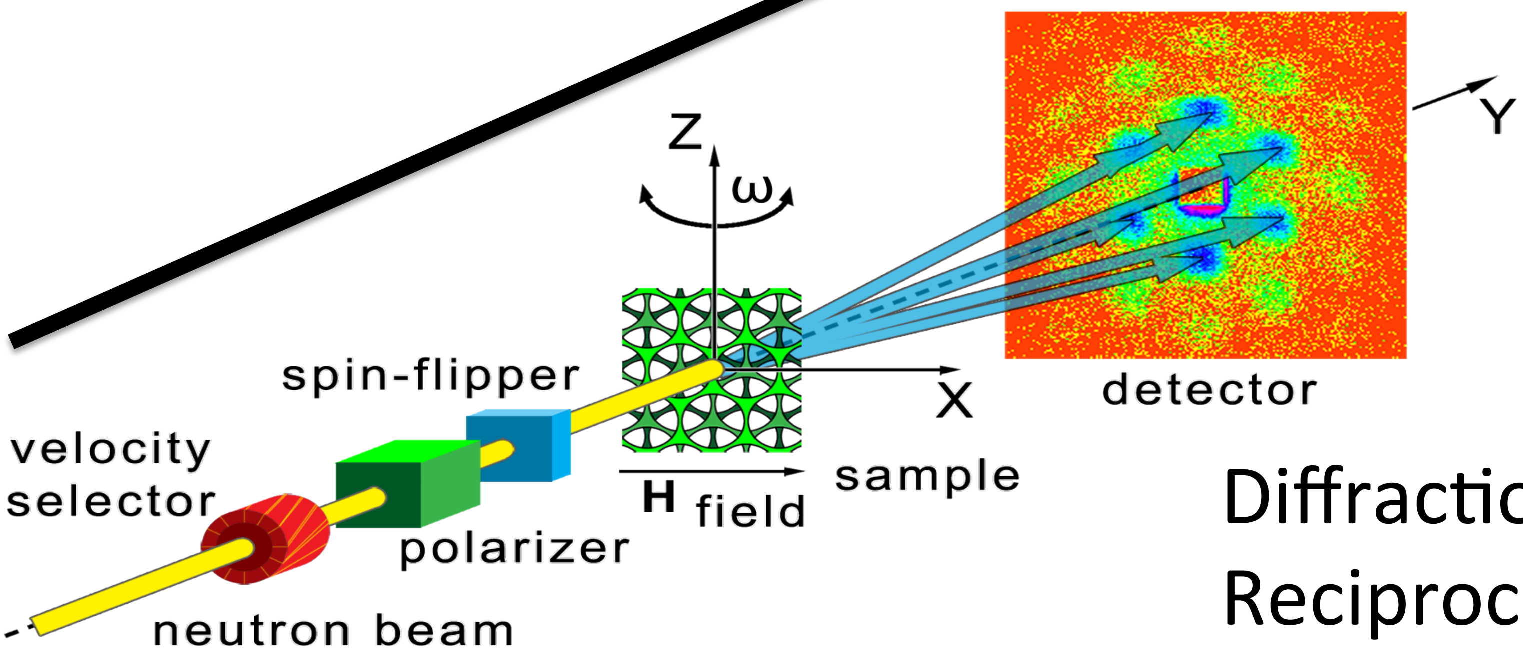
Science 330, 359 (2010)





Microscopy

Real space



Diffraction

Reciprocal space

Course plan

Recap from last week (crystal structure)

Graphene – 2010 Nobel Prize

→ Crystal structures, Lattice vectors, crystal basis etc.

New Goal: Resolve crystal structure of a new 200 K superconductor!

→ Reciprocal space, reciprocal lattice vectors & units, Brillouin zones
→ Scattering theory

Experiments
Scattering triangle
Scattering probability
Bragg's law
Form factor
Structure factor

→ How to resolve crystal structures from scattering experiments

TASKS FOR NEXT WEEK

Tasks for next week

(1) Read chapter 2 :

Braggs Law
Scattering wave amplitude (read fast, don't spend time on the derivation)
Reciprocal Lattice vectors
Diffraction conditions
Laue Equations
Brillouin Zones
Reciprocal lattice (bcc, fcc)
Fourier Analysis of Basis (read fast, don't spend time on the derivation)
Structure factor (bcc,fcc)

(2) Read about: Fermi Golden rule & Fourier transforms

(3) Solve exercise sheet 2

(4) Optional: Install Mathematica

Reciprocal lattice vectors

2-dimensions	3-dimensions
$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$ means $\mathbf{b}_1 \cdot \mathbf{a}_1 = 2\pi$; $\mathbf{b}_1 \cdot \mathbf{a}_2 = 0$ $\mathbf{b}_2 \cdot \mathbf{a}_1 = 0$; $\mathbf{b}_2 \cdot \mathbf{a}_2 = 2\pi$	$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$ $\mathbf{b}_1 = (2\pi/V)\, \mathbf{a}_2 \times \mathbf{a}_3$ $\mathbf{b}_2 = (2\pi/V)\, \mathbf{a}_3 \times \mathbf{a}_1$ $\mathbf{b}_3 = (2\pi/V)\, \mathbf{a}_1 \times \mathbf{a}_2$ $V = \lvert \mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 \rvert$

Exercise 1 *Reciprocal lattice vectors*

a) Show that a reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is orthogonal to the lattice plane (hkl).

b) Show that the distance d_{hkl} of two lattice planes with Miller indices (hkl) is given by

$$d_{hkl} = \frac{2\pi N}{|h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3|}.$$

What is the meaning of N?

Exercise 2 *Reciprocal lattice*

Calculate the primitive reciprocal lattice vectors $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$ for

a) fcc and bcc lattices

b) the hexagonal lattice.

Exercise 3 *Ewald sphere*

Discuss qualitatively, using the Ewald sphere, what kind of interference pattern is observed in the diffraction of monochromatic light by linear point and line lattices.

Exercise 4 *Brillouin zone in the reciprocal lattice*

Construct the first four Brillouin zones for a two-dimensional simple rectangular lattice with $a_2 = 2a_1$.

Exercise 5 *Atomic form factor*

Calculate the atomic form factor f for a homogeneously charged sphere of charge Z and radius R as a function of Δk. Plot f as a function of $\sin(\Theta)$ if we assume $\lambda = R$.

Remember: The atomic form factor for an atom is given by its electron density distribution $n(\vec{r})$ (the charge density is $\rho(\vec{r}) = -en(\vec{r})$) according to

$$f(\Delta\vec{k}) = \iiint n(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} \mathrm{d}^3 r.$$

Furthermore the scattering triangle (figure 1) gives the relation between Δk, the wavelength $\lambda = 2\pi/k$, and the scattering angle Θ:

$$\Delta k = 2 \cdot \frac{2\pi}{\lambda} \sin(\Theta).$$

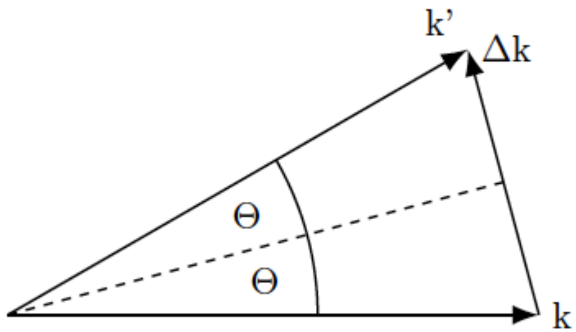


Figure 1: The scattering triangle.

Exercise 6 *Width of the diffraction maximum*

We assume that in a linear crystal on every lattice point $\vec{\rho} = m\vec{a}$, $m \in \mathbb{Z}$, there is an identical point-like scattering centre. The total amplitude of the scattered radiation is proportional to $F = \sum \exp\left(-im\vec{a} \cdot \Delta\vec{k}\right)$. The sum over M lattice points has the value

$$F = \frac{1 - \exp\left(-iM\vec{a} \cdot \Delta\vec{k}\right)}{1 - \exp\left(-i\vec{a} \cdot \Delta\vec{k}\right)}$$

when we use the series expansion

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x}.$$

a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^* F = \frac{\sin^2\left(\frac{1}{2}M\vec{a} \cdot \Delta\vec{k}\right)}{\sin^2\left(\frac{1}{2}\vec{a} \cdot \Delta\vec{k}\right)}.$$

b)For $\vec{a} \cdot \Delta\vec{k} = 2\pi h$, $h \in \mathbb{Z}$, a diffraction maximum appears. We change $\Delta\vec{k}$ slightly and define ε in $\vec{a} \cdot \Delta\vec{k} = 2\pi h + \varepsilon$ such that ε gives the first zero-crossing of the function $\sin\left(\frac{1}{2}M\vec{a} \cdot \Delta\vec{k}\right)$. Show that $\varepsilon = 2\pi/M$. What does this mean for the width of the diffraction maximum?

	Direct Lattice	Reciprocal Lattice	
SC	$\begin{cases}\vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z}\end{cases}$	$\begin{cases}\vec{b}_1 = (2\pi / a)\hat{x} \\ \vec{b}_2 = (2\pi / a)\hat{y} \\ \vec{b}_3 = (2\pi / a)\hat{z}\end{cases}$	SC
FCC	$\begin{cases}\vec{a}_1 = \frac{1}{2}a(\hat{x}+\hat{y}) \\ \vec{a}_2 = \frac{1}{2}a(\hat{y}+\hat{z}) \\ \vec{a}_3 = \frac{1}{2}a(\hat{z}+\hat{x})\end{cases}$	$\begin{cases}\vec{b}_1 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})\end{cases}$	BCC
BCC	$\begin{cases}\vec{a}_1 = \frac{1}{2}a(\hat{x}+\hat{y}-\hat{z}) \\ \vec{a}_2 = \frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{a}_3 = \frac{1}{2}a(\hat{x}-\hat{y}+\hat{z})\end{cases}$	$\begin{cases}\vec{b}_1 = \frac{2\pi}{a}(\hat{x}+\hat{y}) \\ \vec{b}_2 = \frac{2\pi}{a}(\hat{y}+\hat{z}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{z}+\hat{x})\end{cases}$	FCC