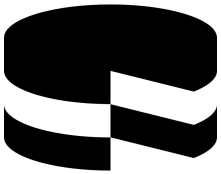
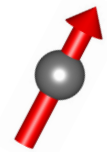
Spaces of crystallography: Reciprocal lattice

synchrotron x-ray diffraction



aperiodic crystals

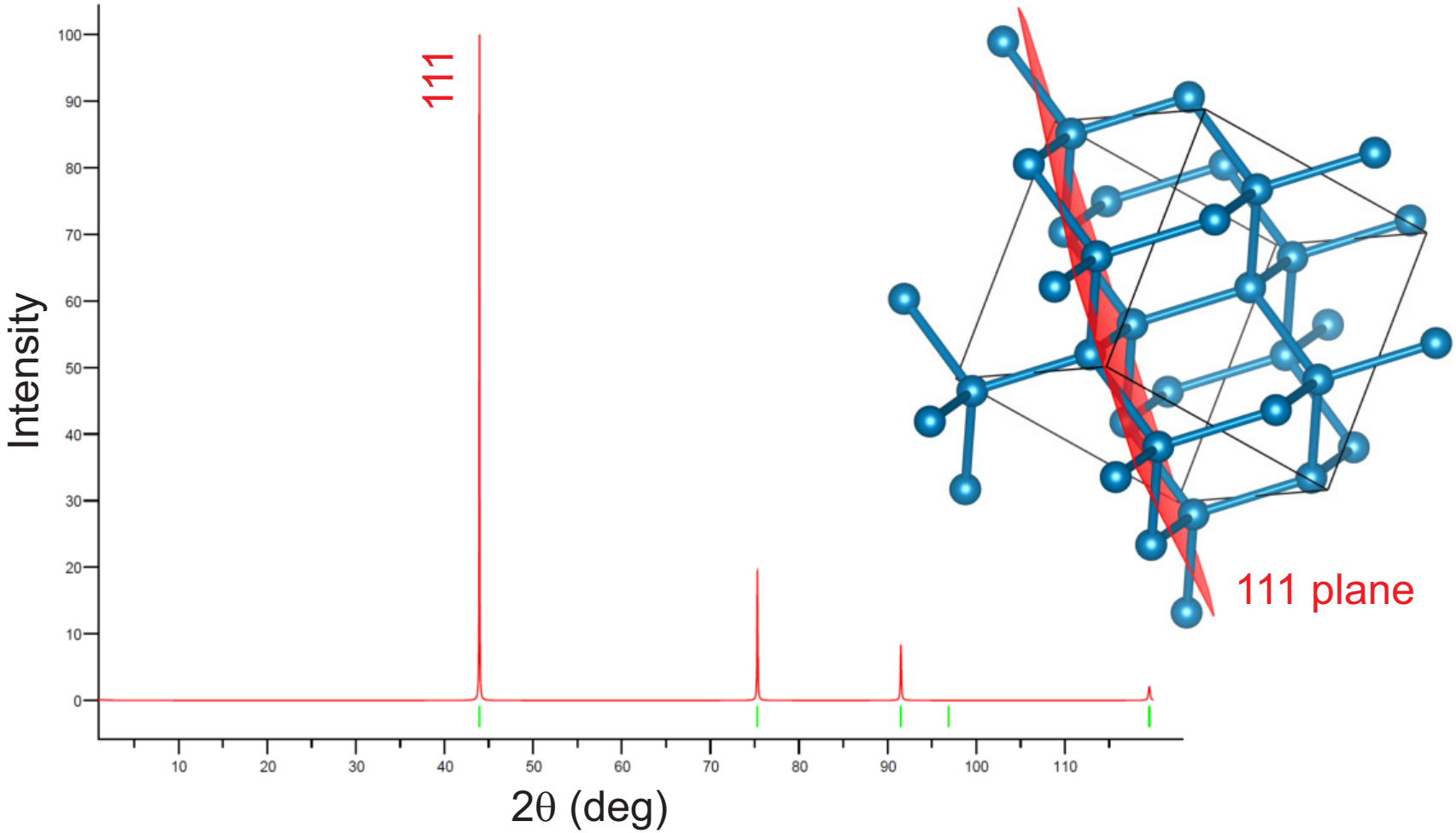
Max Laue and Paul Ewald



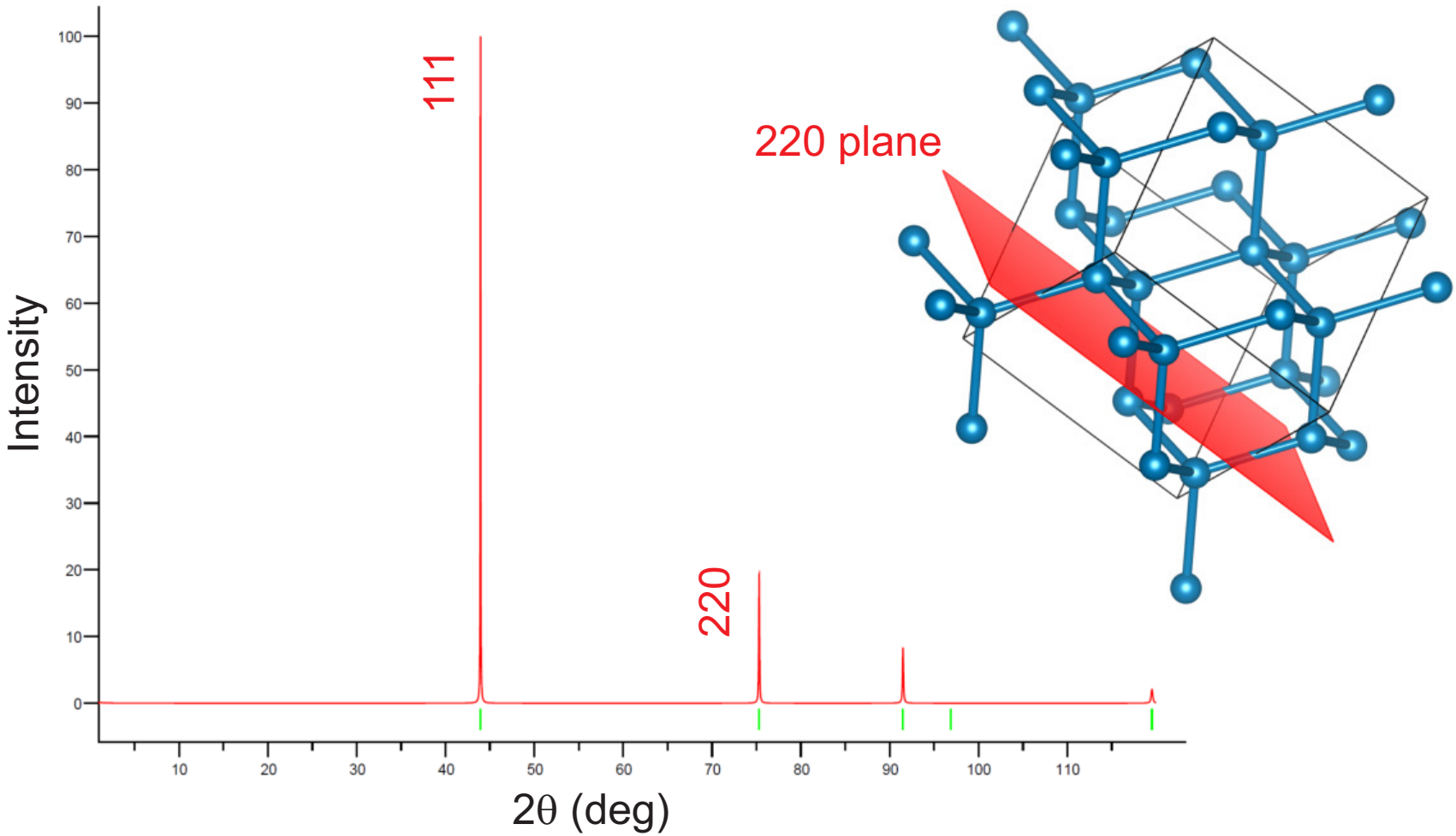
by Alexander Tsirlin, Leipzig University

Lecture 5: October 25, 2023

Problem of lattice planes



Problem of lattice planes



Lattice planes may not contain any atoms, yet they scatter x-rays

Person

Max Laue and Paul Ewald

Max von Laue
1879–1960

- 1899–1903: university study (mathematics, physics) in Strasbourg, Göttingen, Berlin, and Munich
- 1903: PhD obtained under Max Planck
- 1904–05: more study in Göttingen (chemistry), teacher's certificate
- 1906–09: Privatdozent in Berlin
- 1902–12: Privatdozent in Munich

"...one lived there in an atmosphere saturated with problems concerning the specific nature of X-rays"

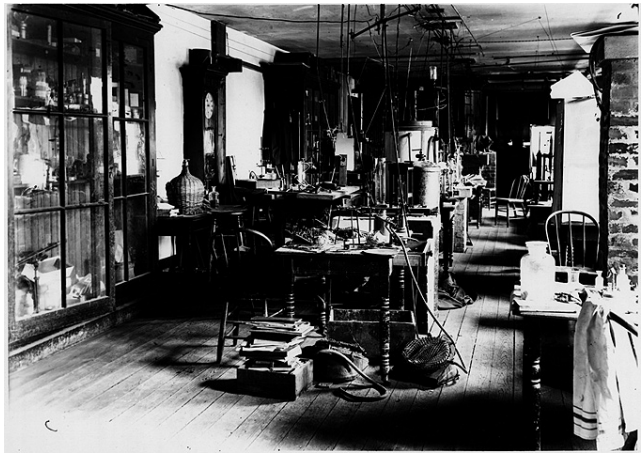
Wilhelm Röntgen
experiment

Arnold Sommerfeld
theory

University of Munich (present LMU)

Wilhelm Röntgen
experiment

own laboratory

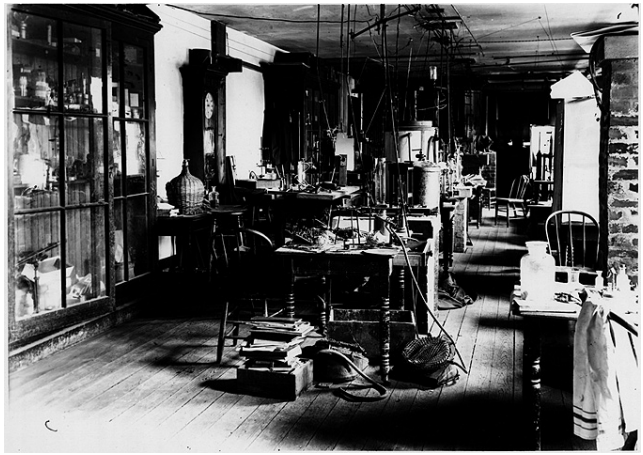


Arnold Sommerfeld
theory

University of Munich (present LMU)

Wilhelm Röntgen
experiment

own laboratory



Arnold Sommerfeld
theory

Cafe Lutz, meeting place in Hofgarten

Max von Laue
1879–1960

Paul Ewald
1888–1985

Ewald's PhD thesis (1912):

Propagation of visible light in anisotropic crystals

Max von Laue
1879–1960

Paul Ewald
1888–1985

Ewald's PhD thesis (1912):

Propagation of visible light in anisotropic crystals

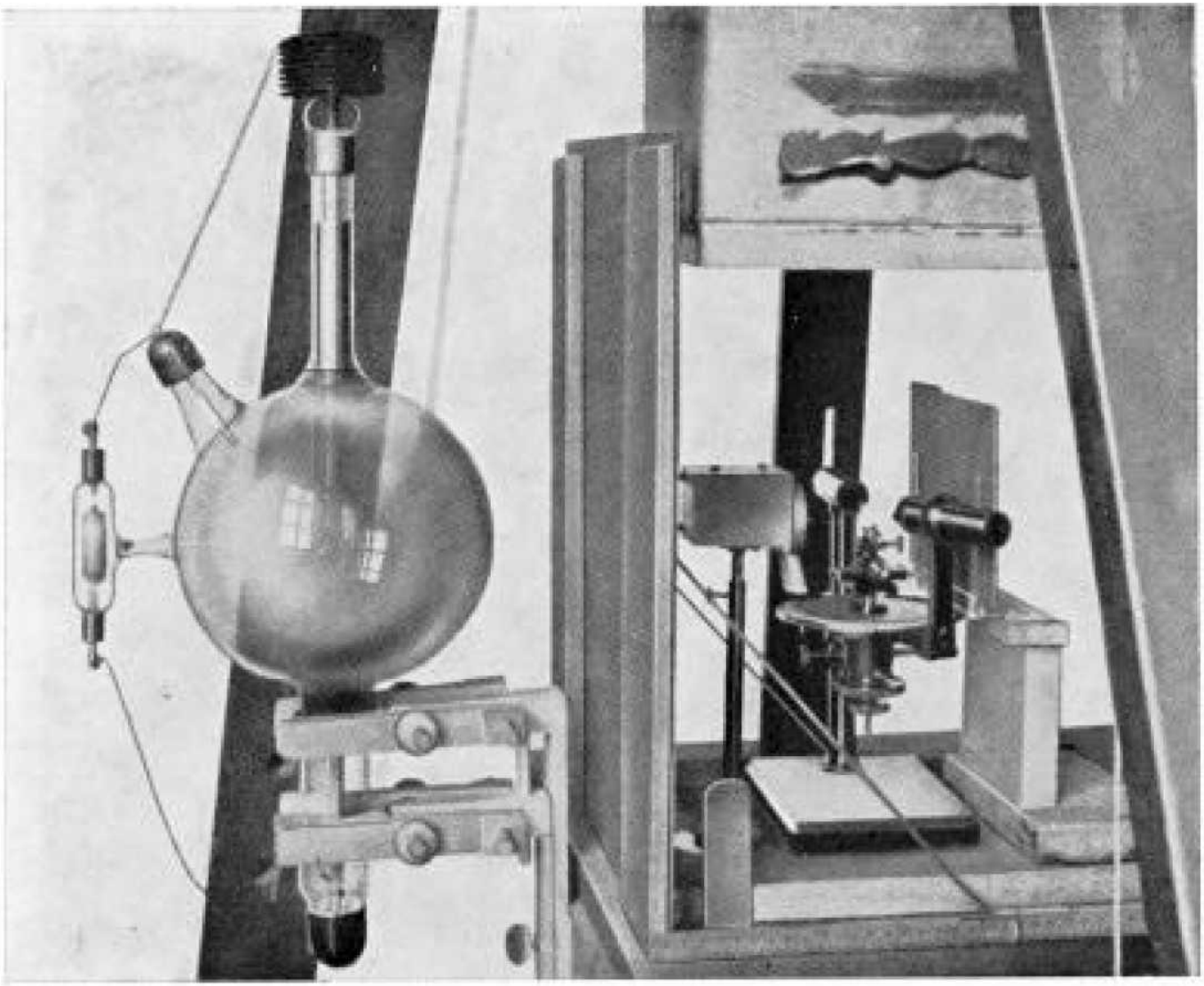
Laue:

What would happen if you assumed very much shorter waves to travel in the crystal?

Ewald:

This formula from my thesis is also valid for short wavelengths. I, however, have to get my thesis delivered within the next few days... You are welcome to discuss the formula yourself.

Very first diffraction experiment



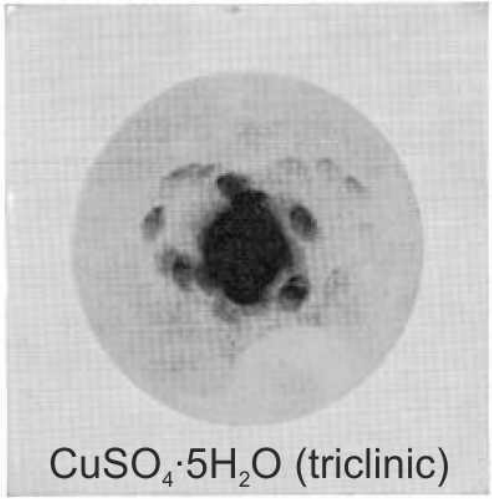
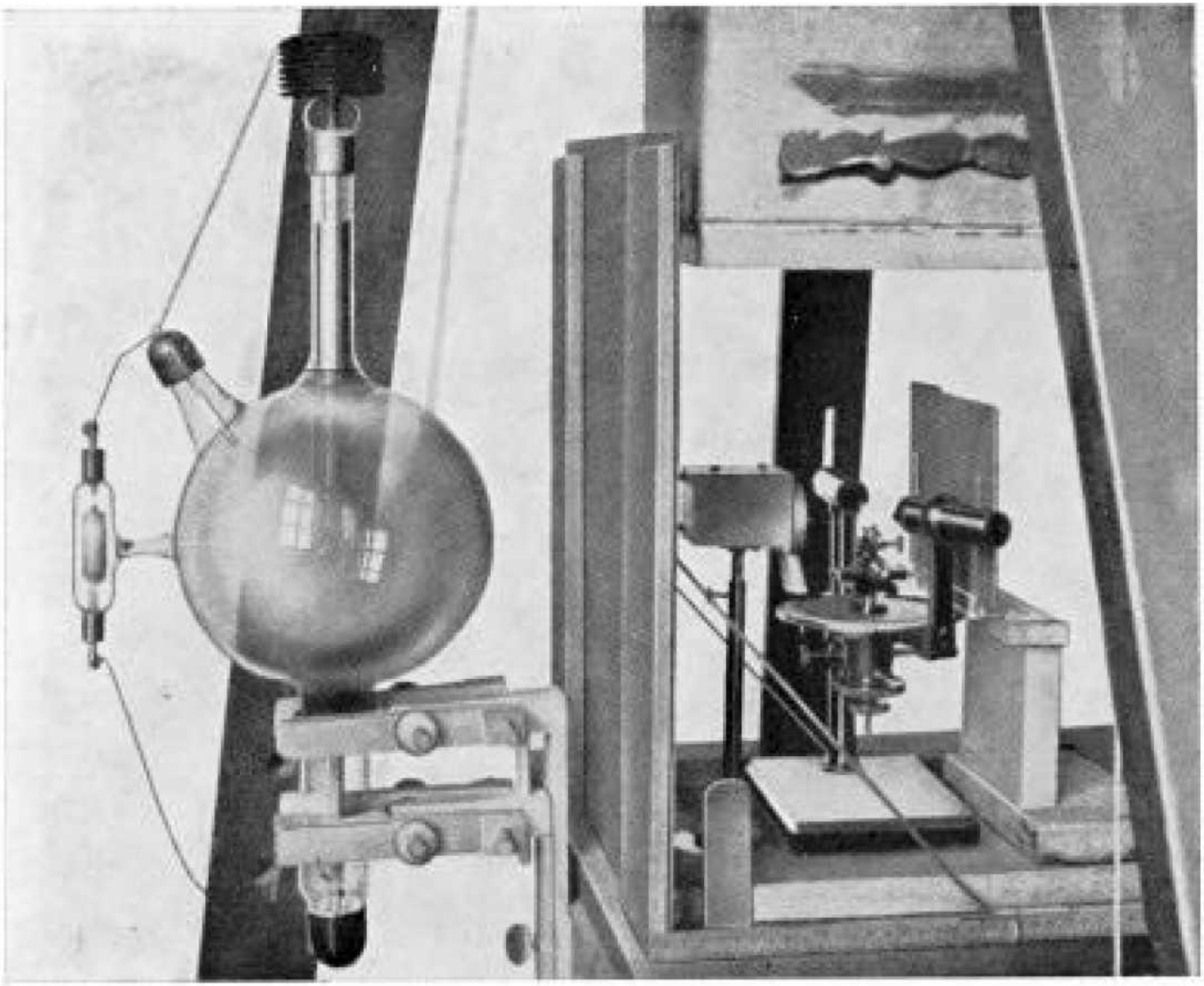
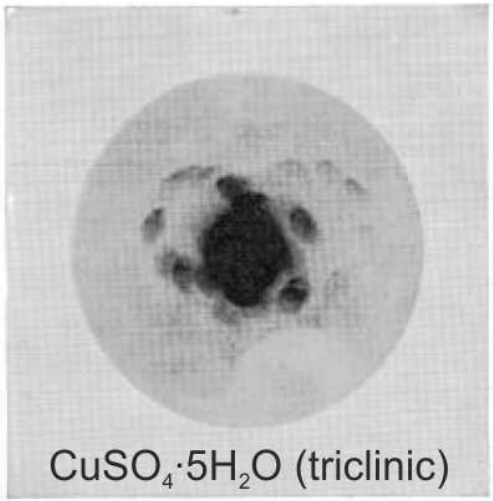


Image credit: 50 years of x-ray diffraction

Very first diffraction experiment





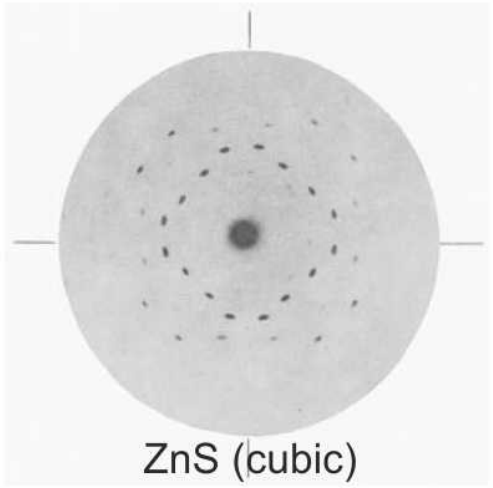
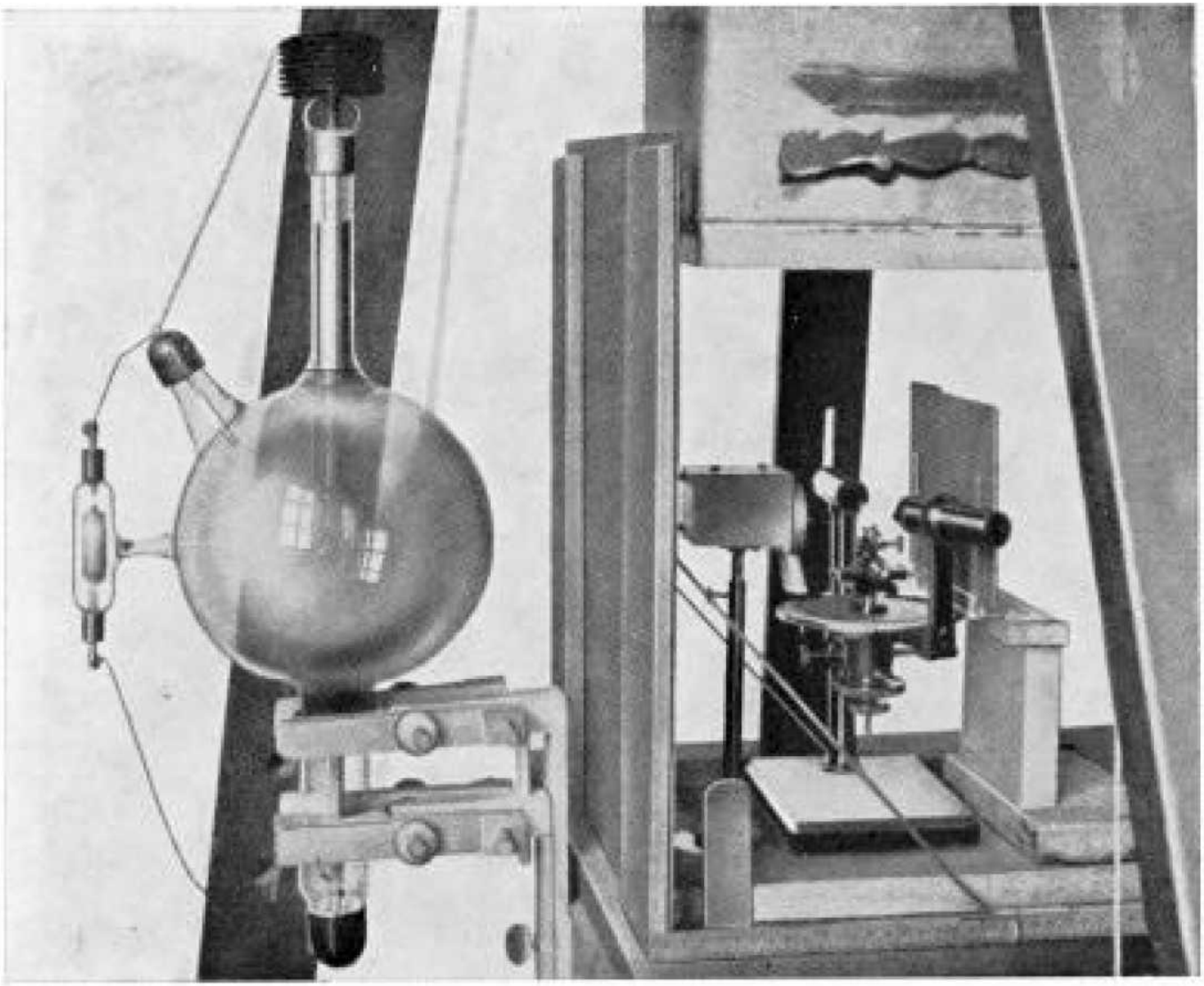
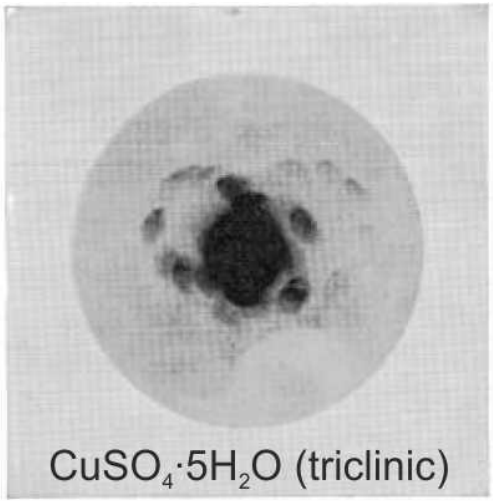
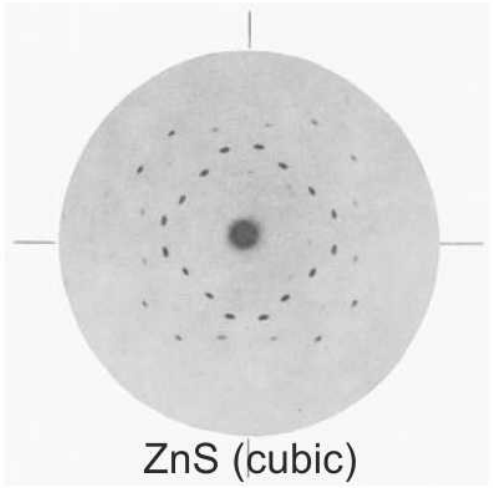


Image credit: 50 years of x-ray diffraction

Very first diffraction experiment



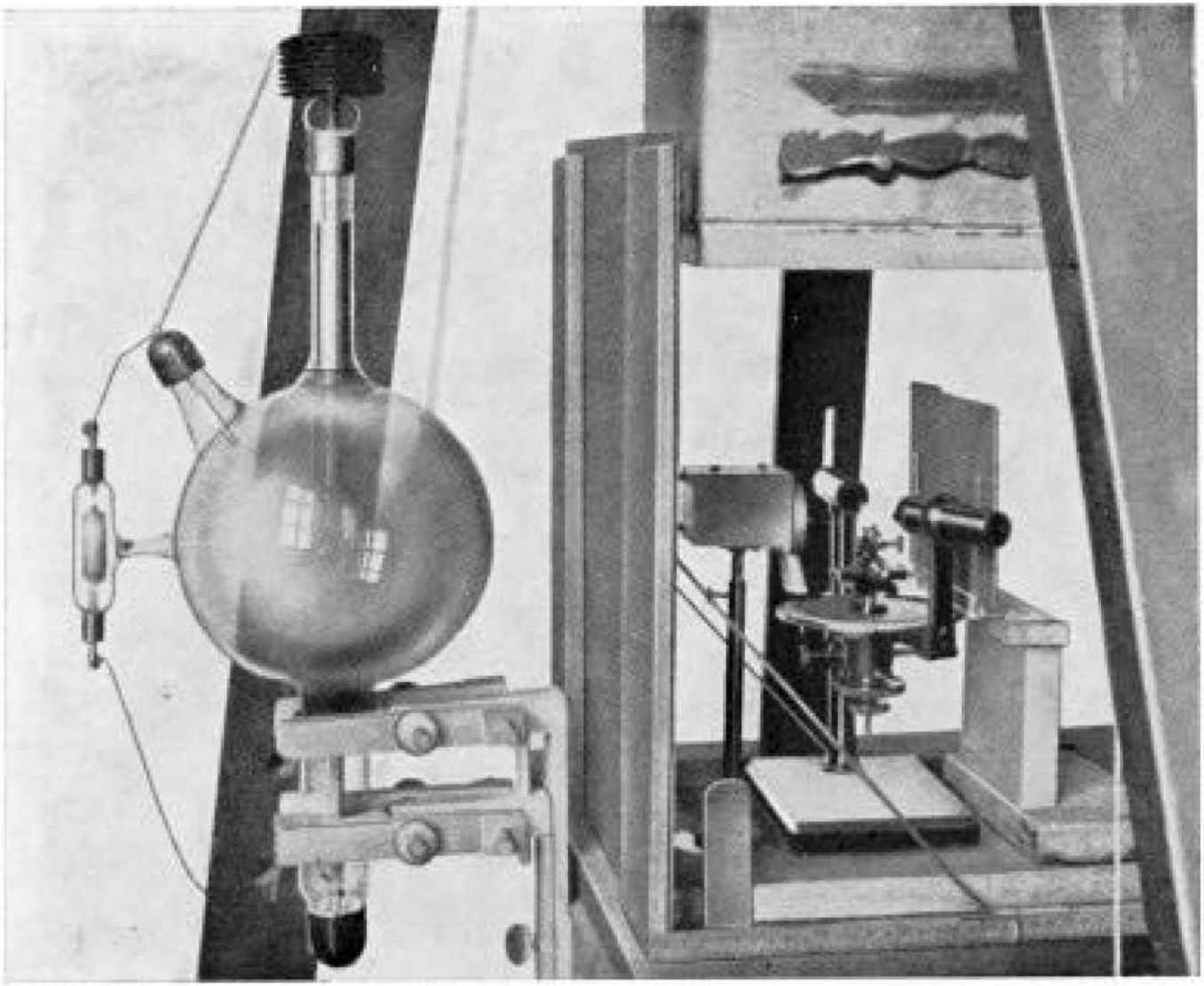


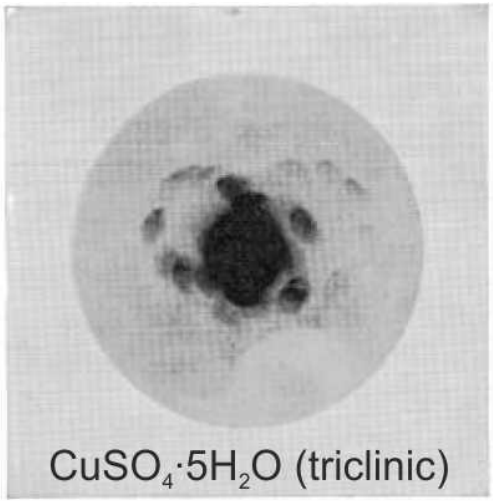


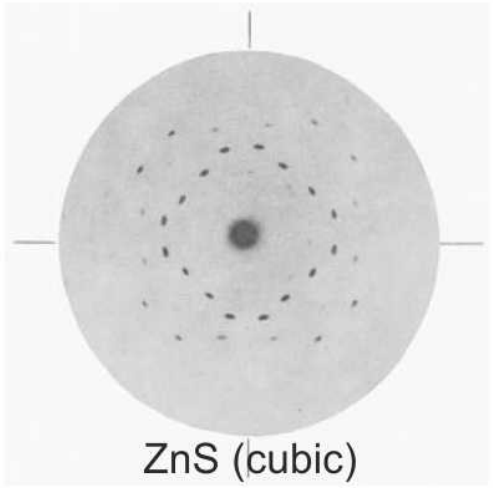
Nobel prize: 1914 – Laue

Image credit: 50 years of x-ray diffraction

Very first diffraction experiment







Nobel prize: 1914 – Laue, 1915 – Braggs...

Image credit: 50 years of x-ray diffraction

In German, *Gitter* means 'lattice', but also 'fence'

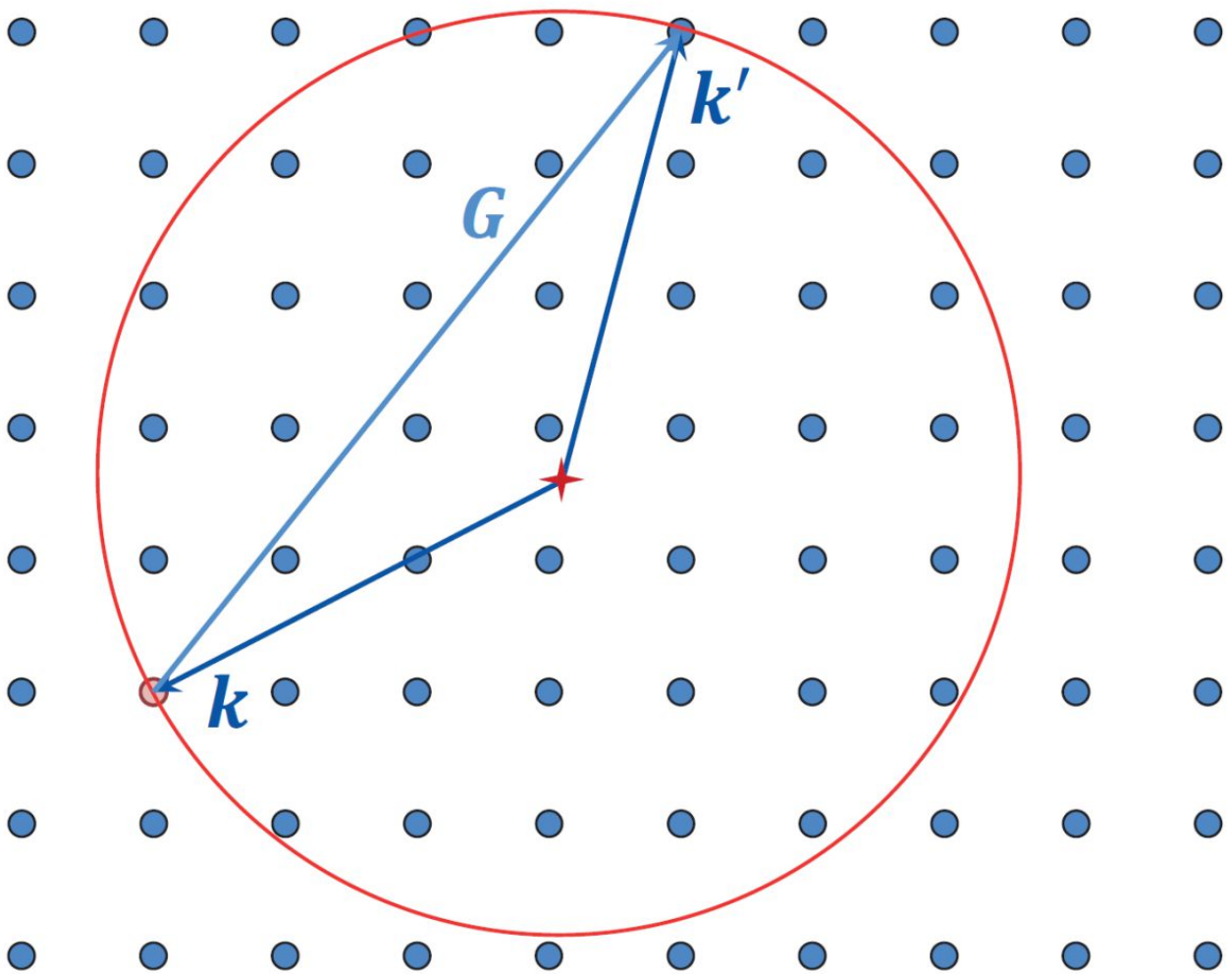
direktes Gitter
protects your house
from strangers

In German, *Gitter* means 'lattice', but also 'fence'

direktes Gitter
protects your house
from strangers

reziprokes Gitter
lures people in

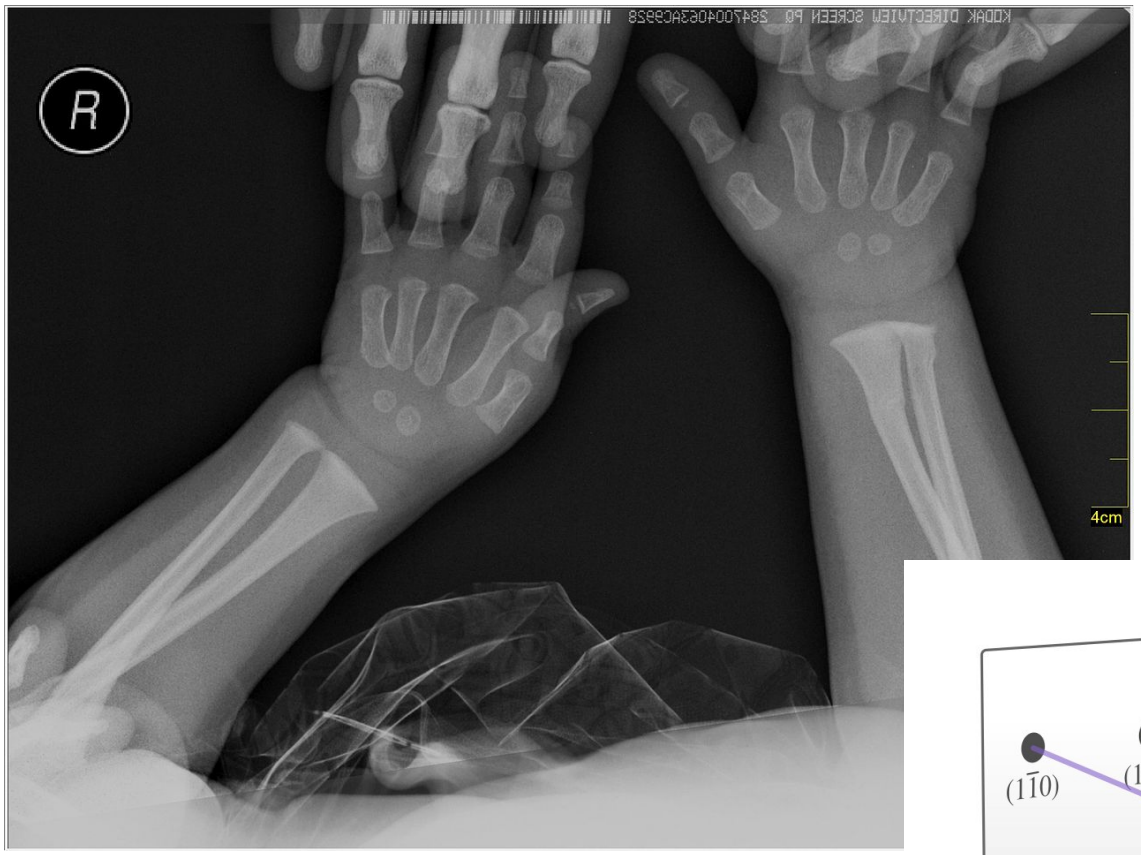
Ewald sphere



Radius determined by radiation wavelength, $|\boldsymbol{k}| = 2\pi/\lambda$

Image from Gross and Marx, Festkörperphysik

X-ray image of a crystal



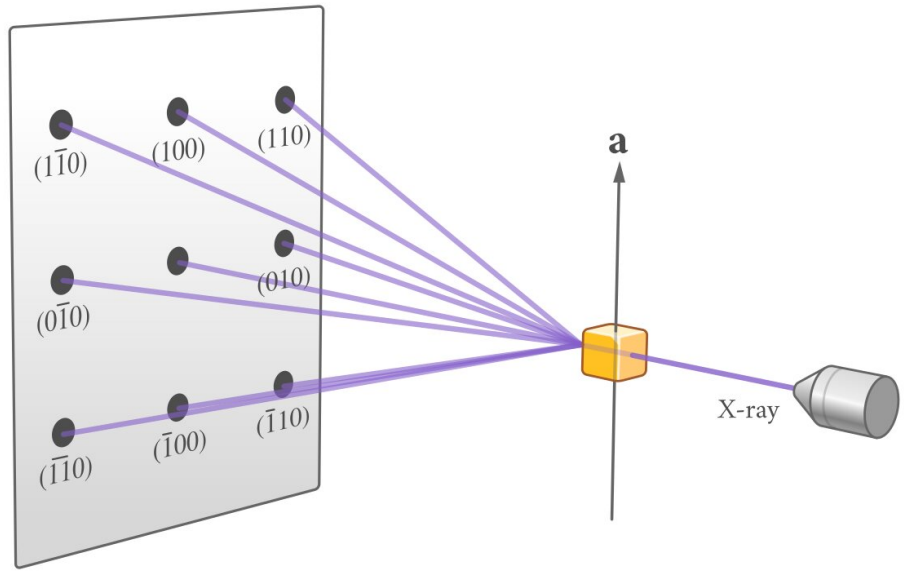
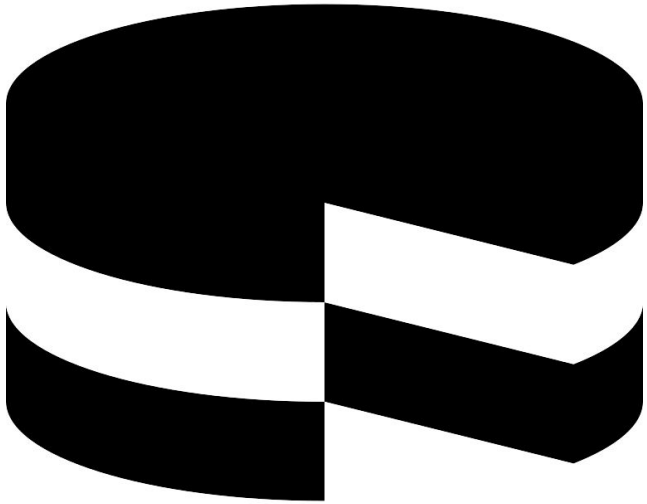


Image credits: Nevit Dilmen and LibreTexts Chemistry (CC-BY-SA)



Material

aperiodic crystals

Strange diffraction patterns

Na_2CO_3
washing soda

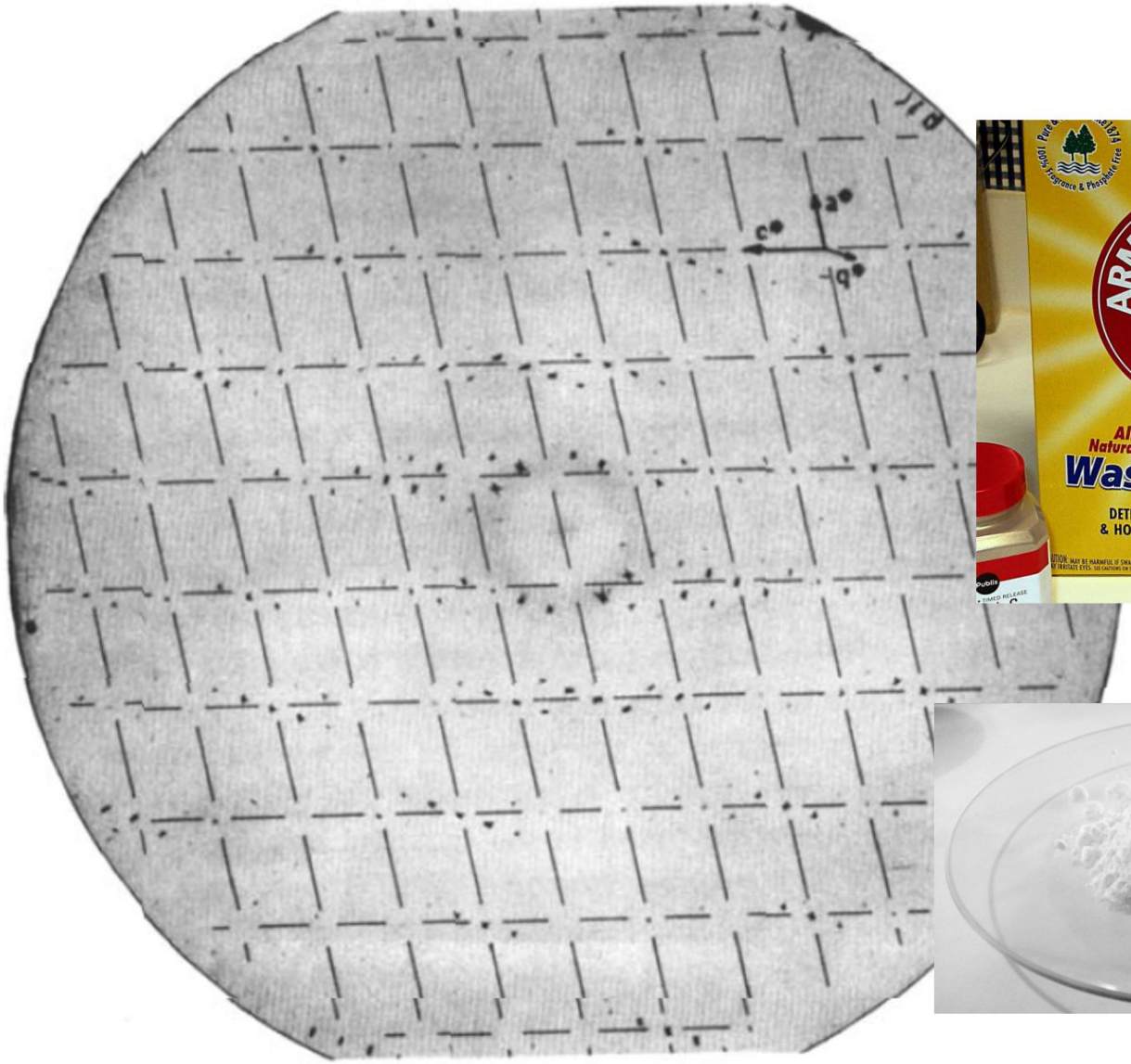


Image credits: Acta Cryst. B32, 47 (1976), Caffenol (CC-BY-NC), public domain

$AuTe_2$, known since 1861

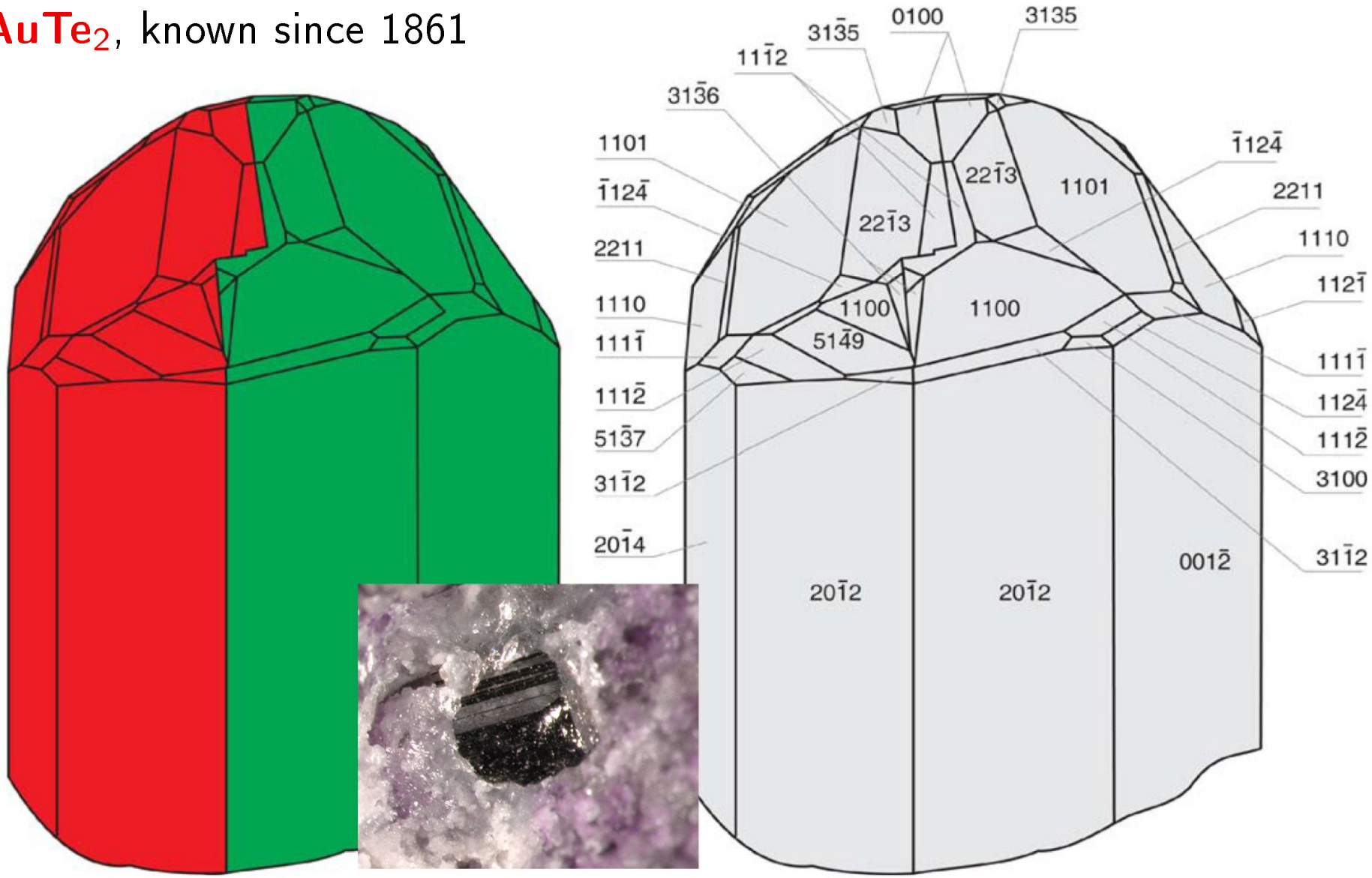
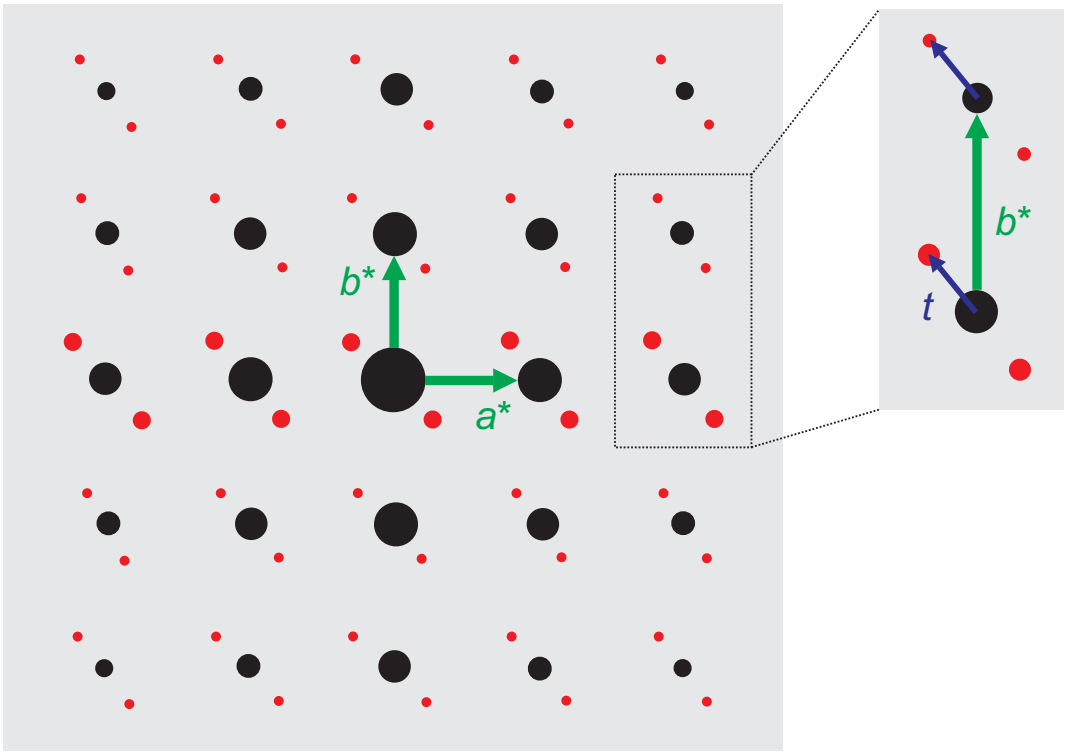


Image credit: Cryst. Eng. 6, 187 (2003) and Robert Lavinsky (CC-BY-SA)

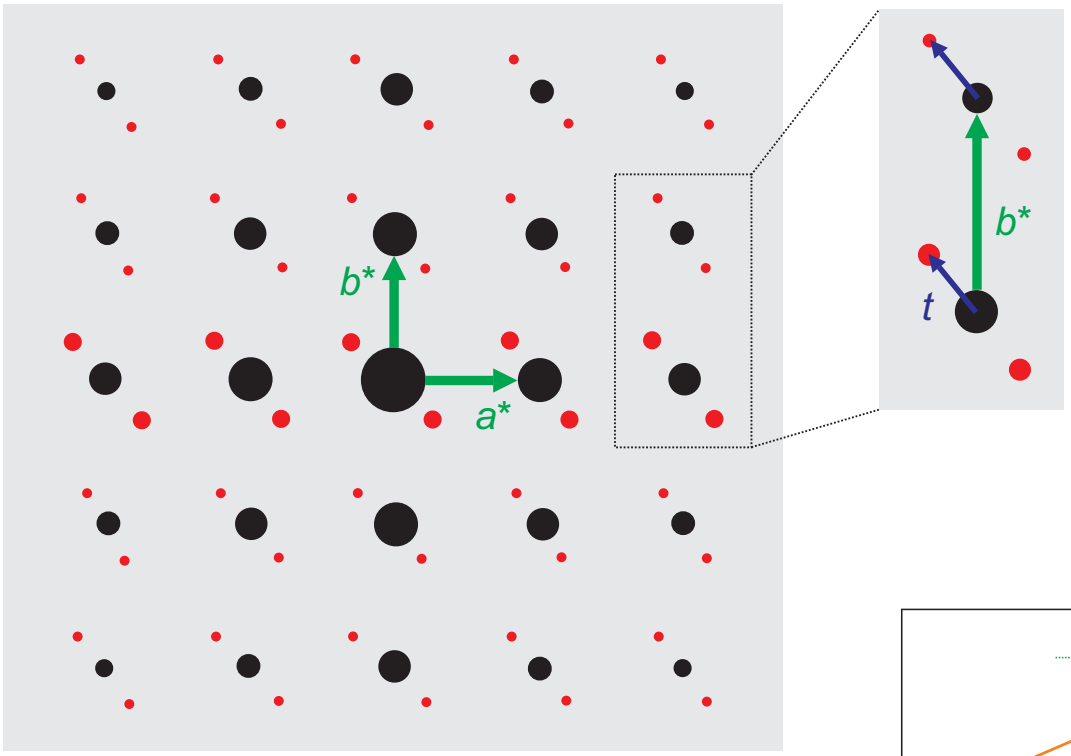


main reflections satellites

modulation vector

Reciprocal space

h, k, l + index along t
(4D space)

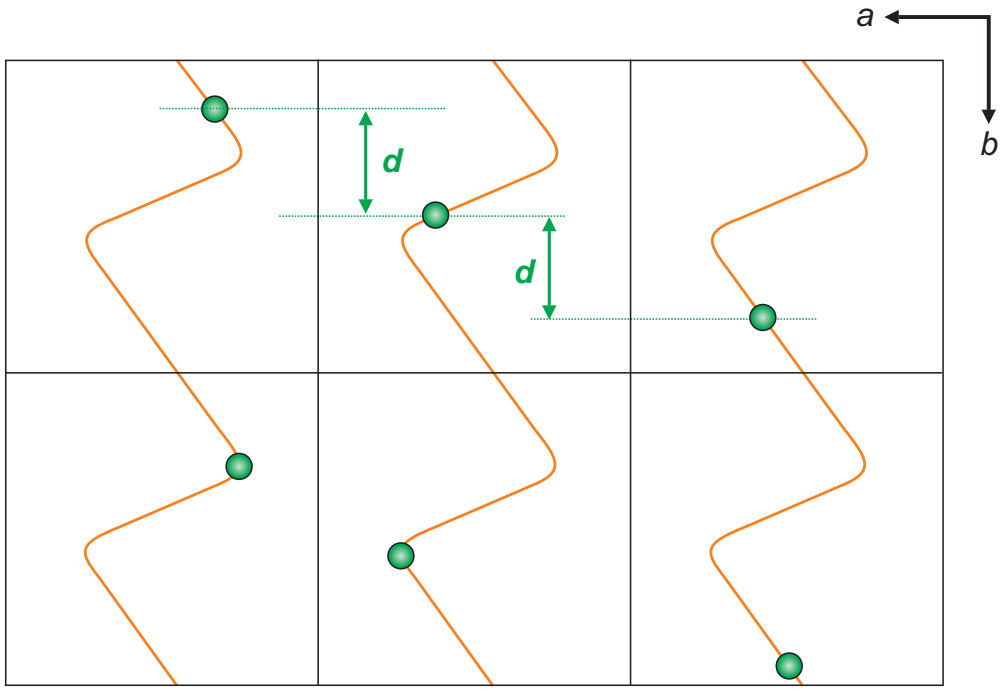


Reciprocal space

h, k, l + index along t
(4D space)

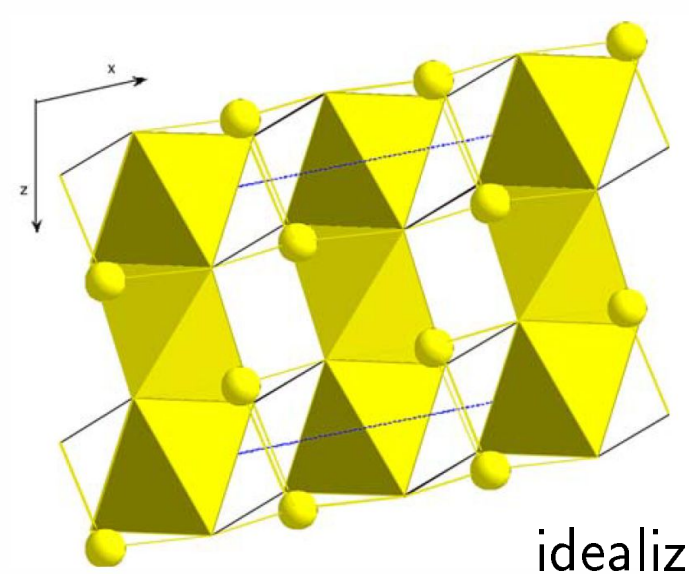
main reflections satellites

modulation vector

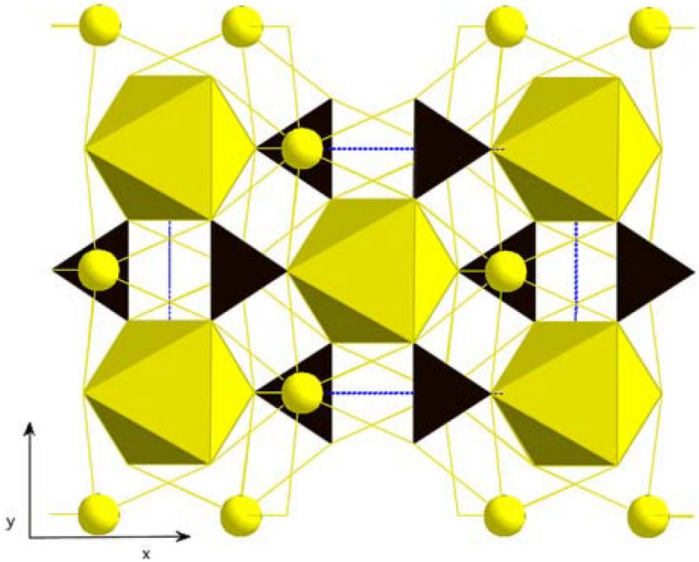


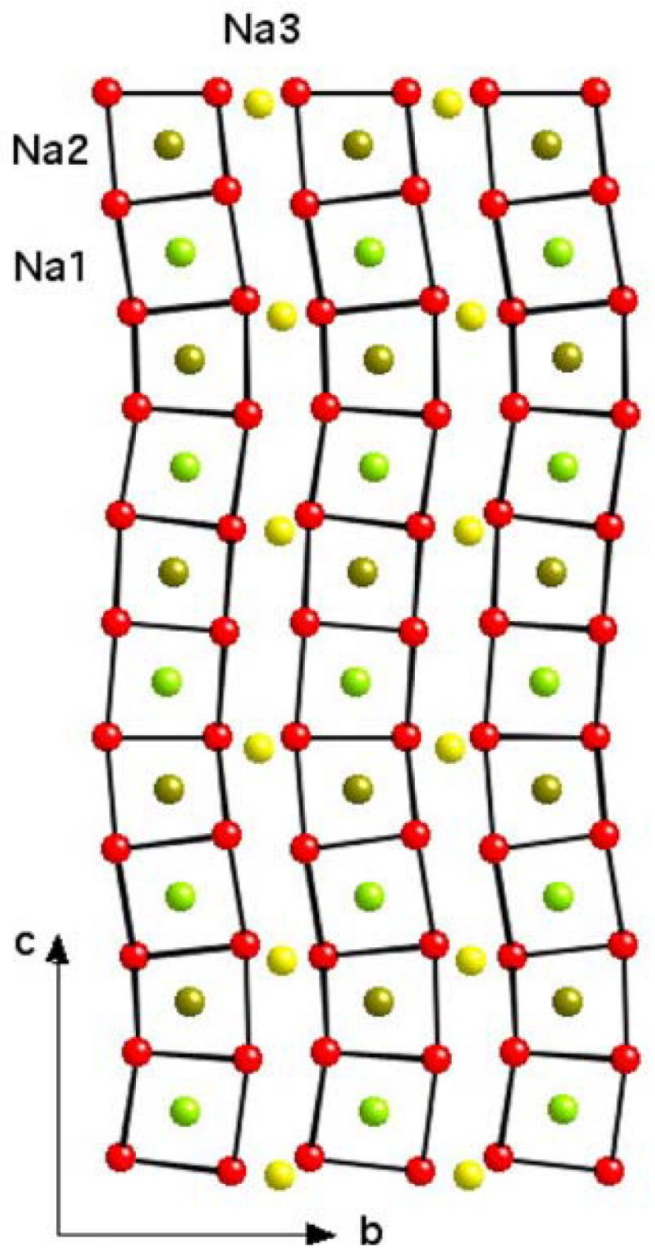
Direct space

Na_2CO_3 structure



idealized structure (3D)





real structure ("4D")

Image credit: Cryst. Eng. 6, 187 (2003)

International Union of Crystallography

Report of the Executive Committee for 1991

Crystal is any solid having an essentially discrete diffraction pattern

Aperiodic crystal is any crystal in which 3D periodicity is absent

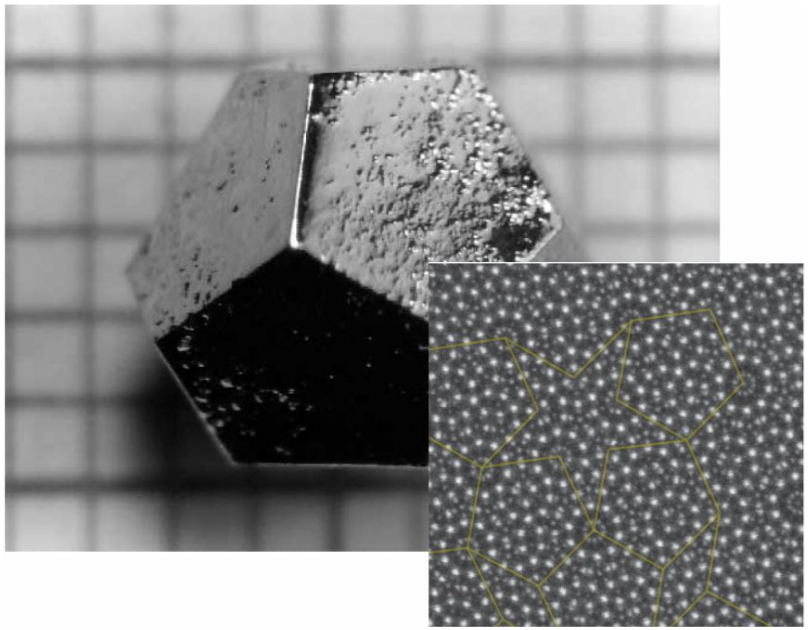
International Union of Crystallography

Report of the Executive Committee for 1991

Crystal is any solid having an essentially discrete diffraction pattern

Aperiodic crystal is any crystal in which 3D periodicity is absent

Quasicrystals are aperiodic crystals



Experimental technique

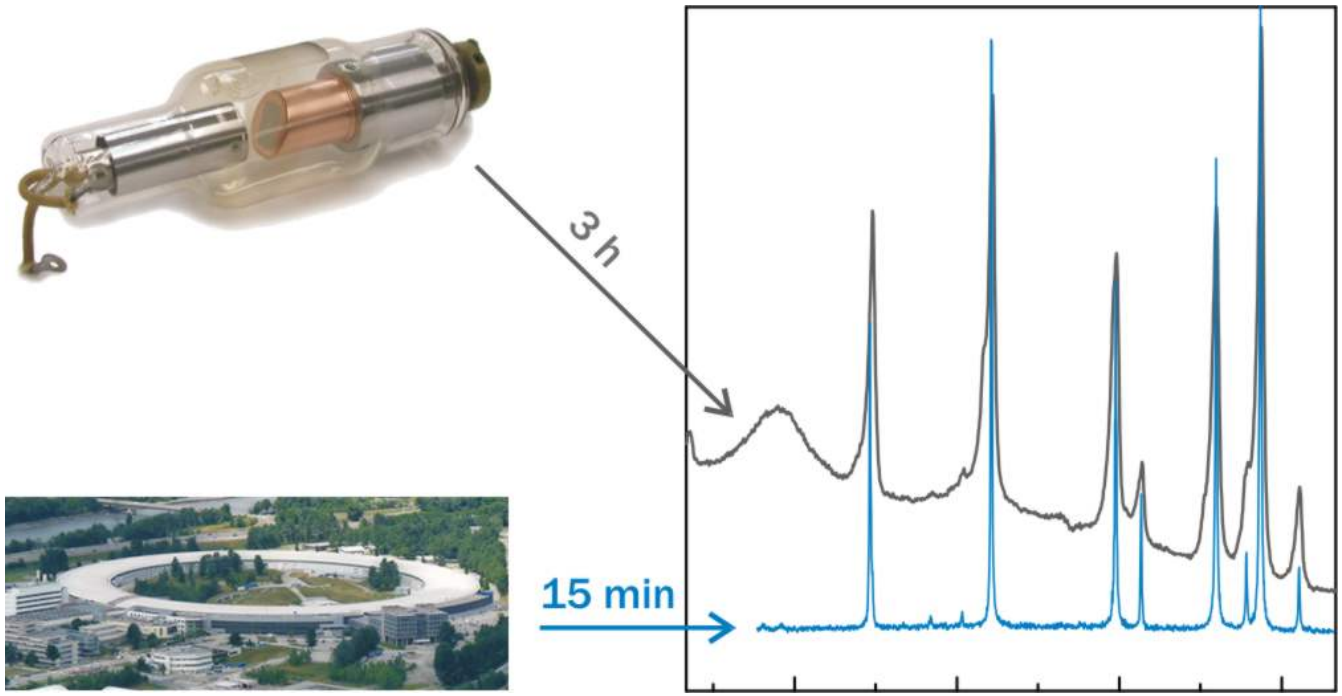
synchrotron x-ray diffraction

- **Sealed x-ray tube:**
  flux $= 5 \times 10^9$ photons/s m^2
  cheap, robust, easy to use

- **Rotating anode:**
  flux $= 5 \times 10^{10}$ photons/s m^2
  available in the lab,
  but still fixed wavelength

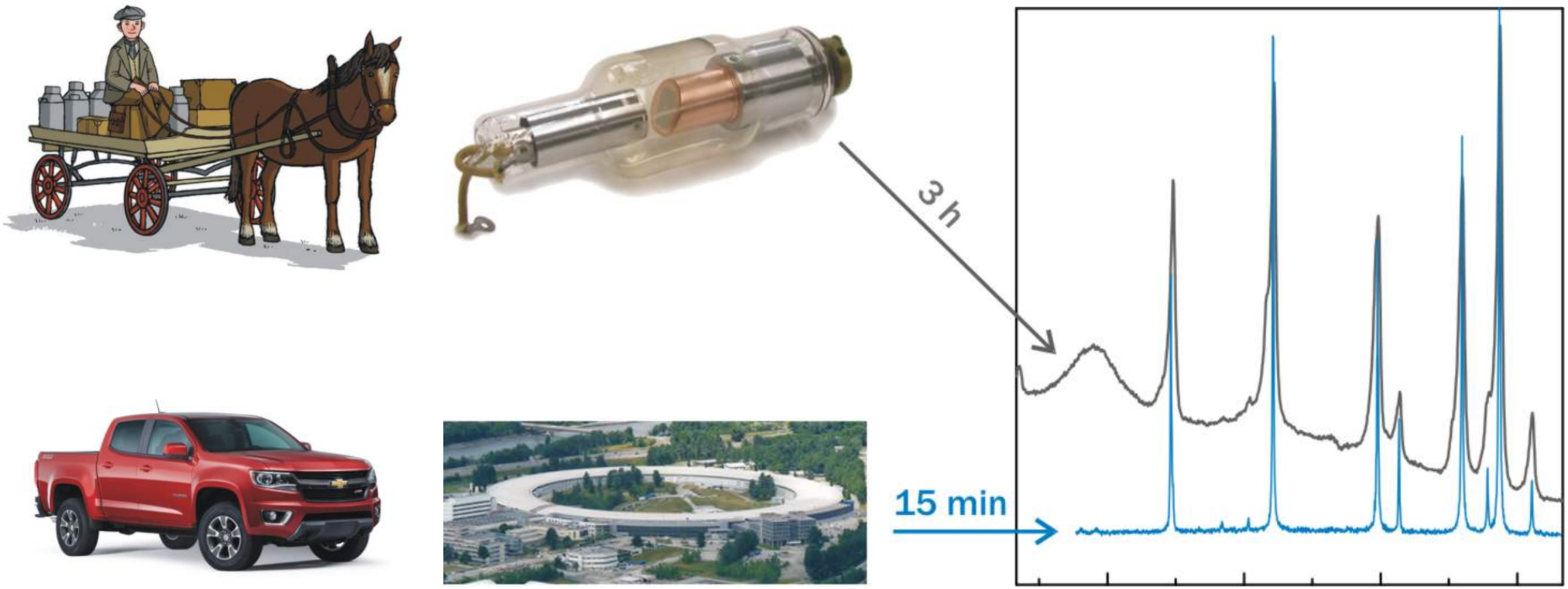
- **Synchrotron:**
  flux $= 10^{17} - 10^{24}$ photons/s m^2
  broad energy spectrum,
  but requires a large-scale facility

Synchrotron diffraction



- Resolution and signal-to-noise ratio largely improved
- Fast data collection
- Specialized sample environments: high pressure, *in situ* (batteries, reactors), etc.

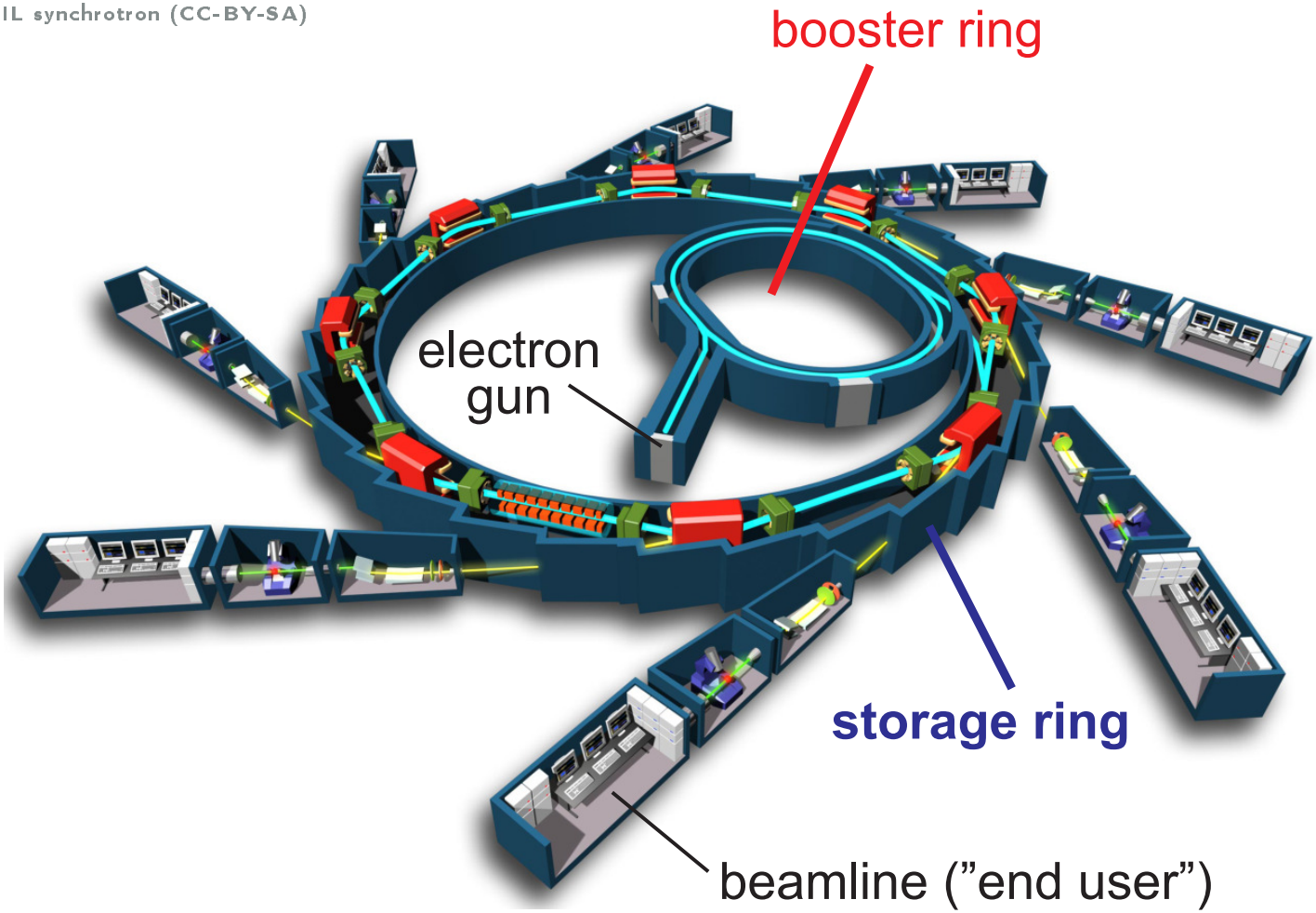
Synchrotron diffraction



- Resolution and signal-to-noise ratio largely improved
- Fast data collection
- Specialized sample environments: high pressure, *in situ* (batteries, reactors), etc.

Circles of light

Image credit: SOLEIL synchrotron (CC-BY-SA)



Booster ring accelerates electrons to 2 – 6 GeV

Storage ring maintains constant current of 150 – 200 mA

Storage ring

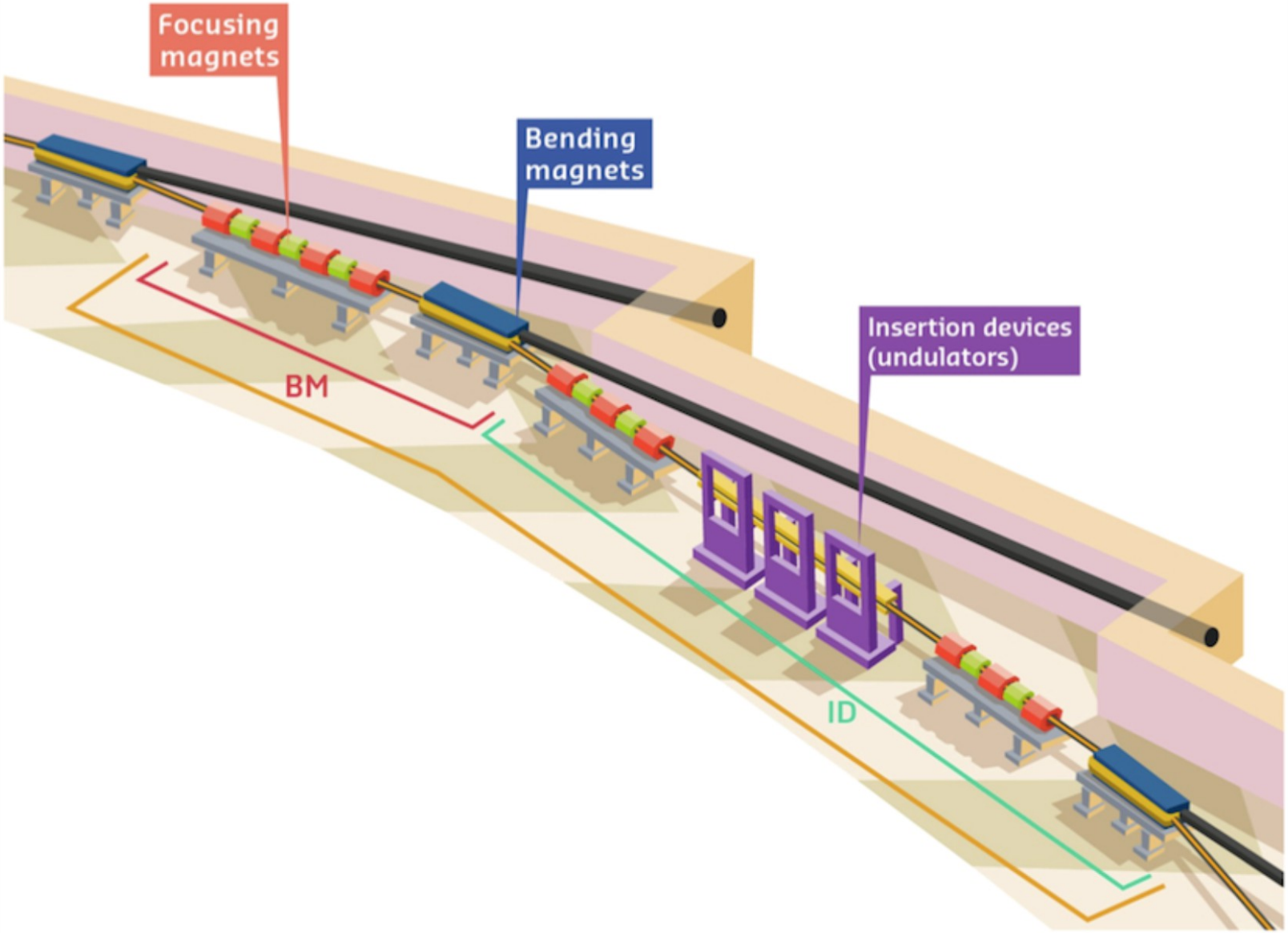


Image credit: ESRF

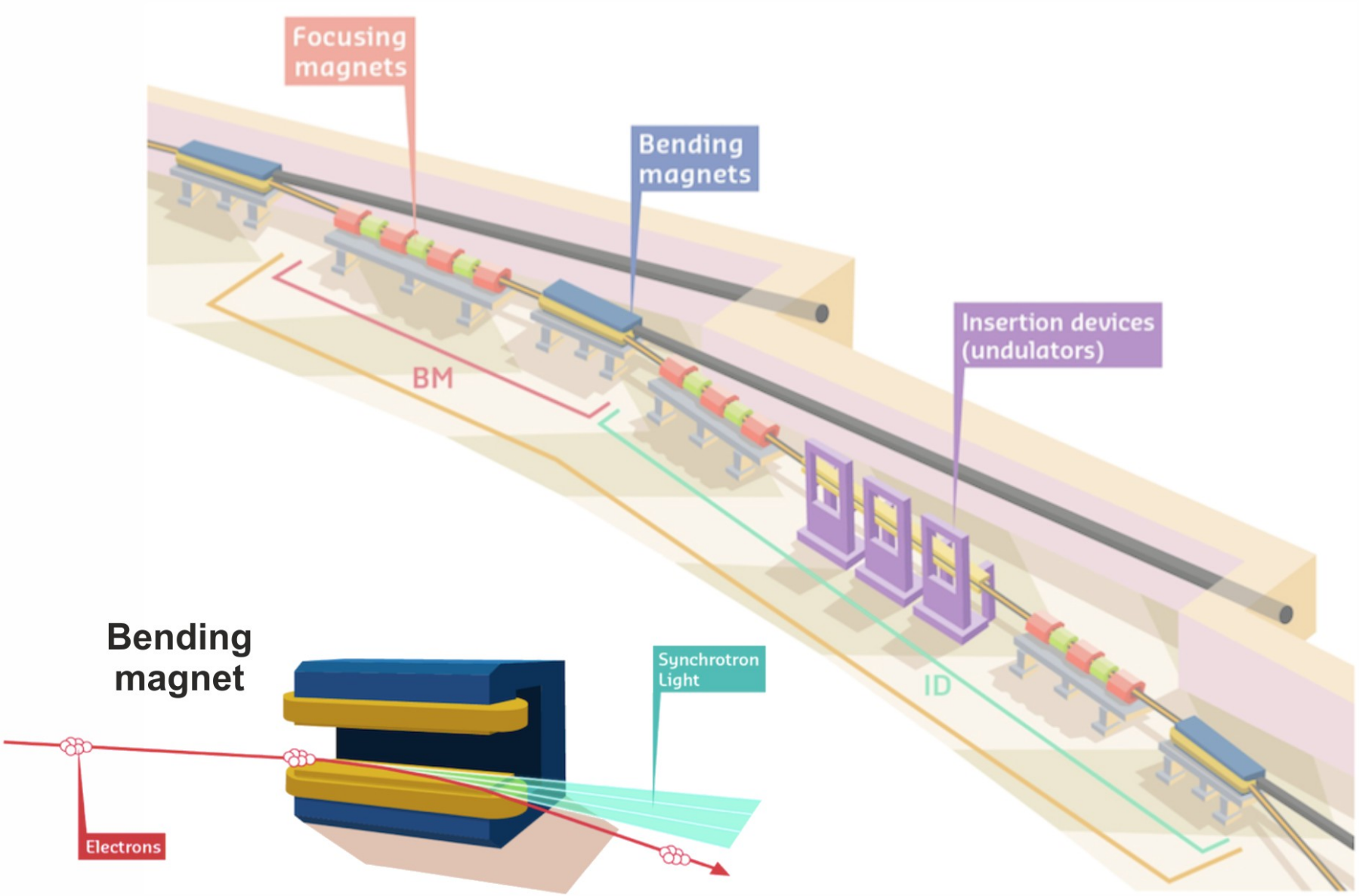


Image credit: ESRF

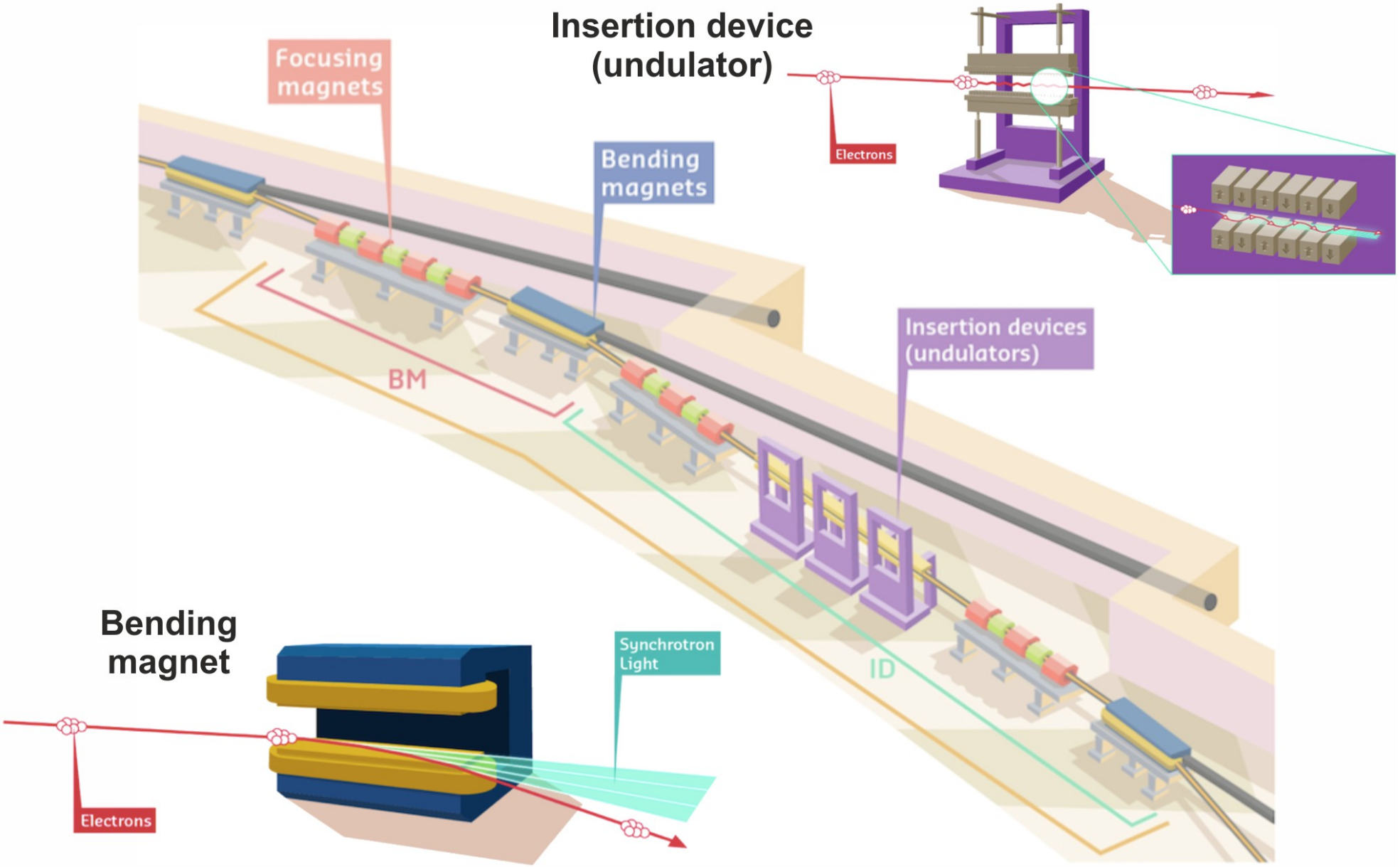
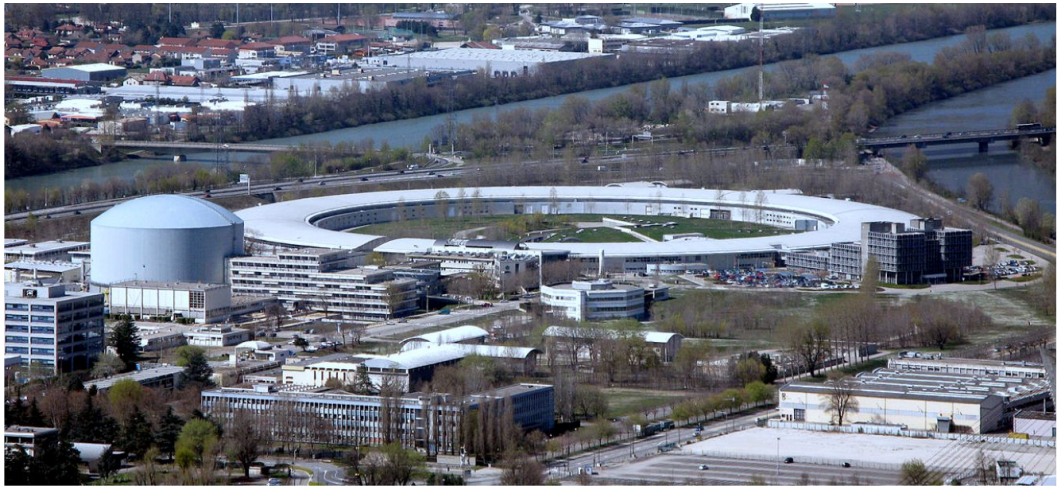
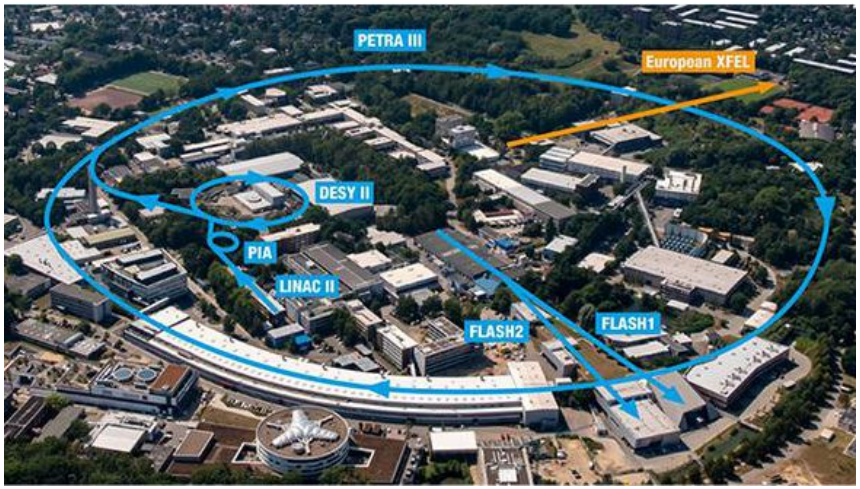


Image credit: ESRF

ESRF (844 m)
Grenoble, France



PETRA-III (2 300 m)
Hamburg, Germany



SOLEIL (354 m)
Orsay, France

Image credits: Rama and SOLEIL (CC-BY-SA) + DESY (fair use)

Synchrotrons in Europe

Image credit: ESRF