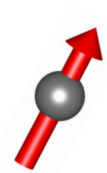
Magnetic crystallography

propagation vector, magnetic symmetry

neutron diffraction

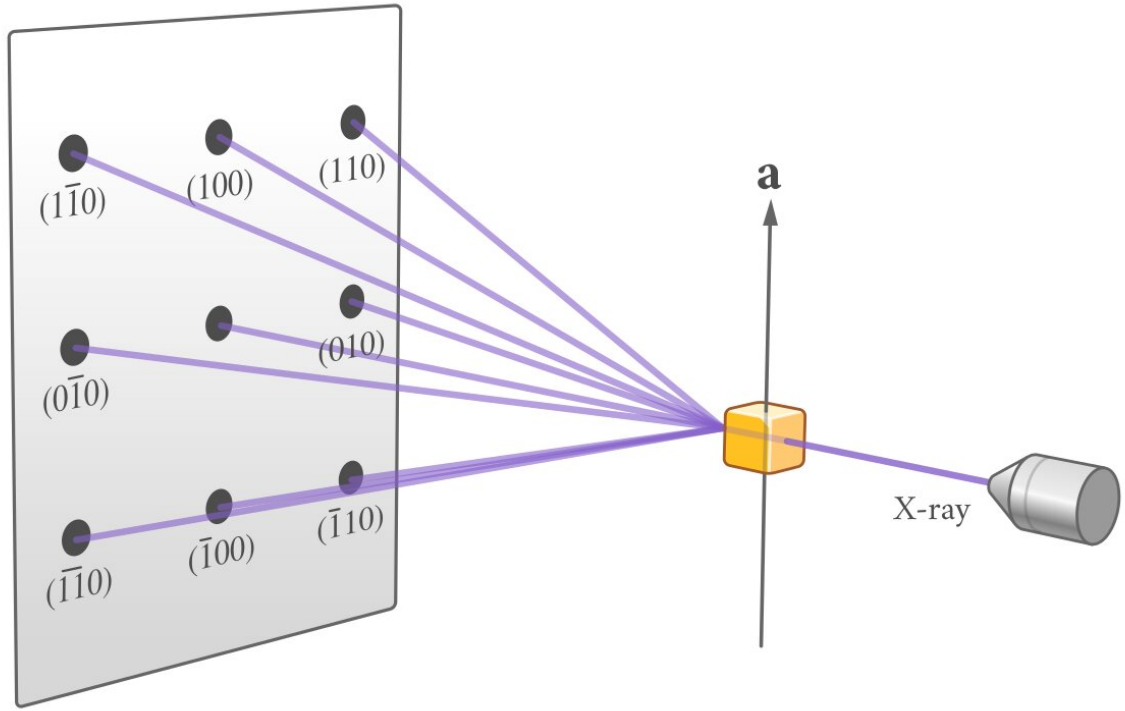
Clifford Shull



by Alexander Tsirlin, Leipzig University

Lecture 7: December 16, 2024

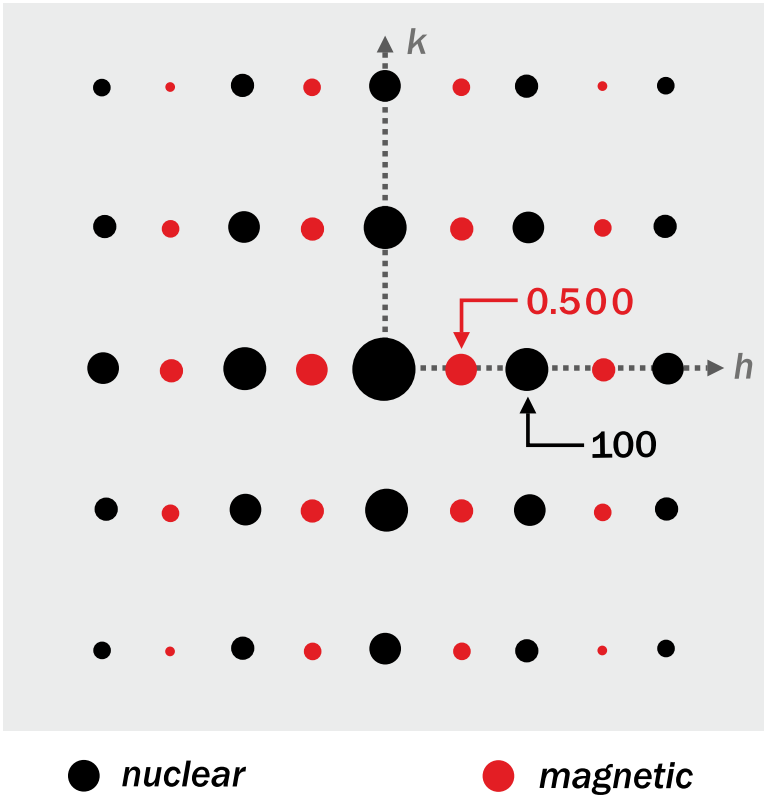
“Philosophy” of diffraction experiments

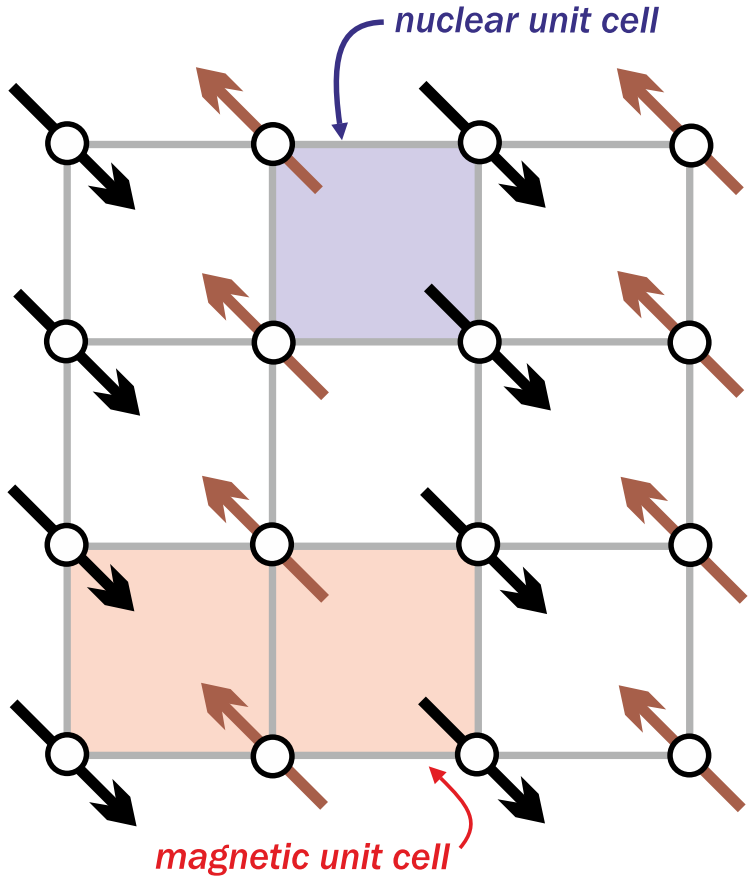


Positions of reflections $\longrightarrow$ **lattice parameters**

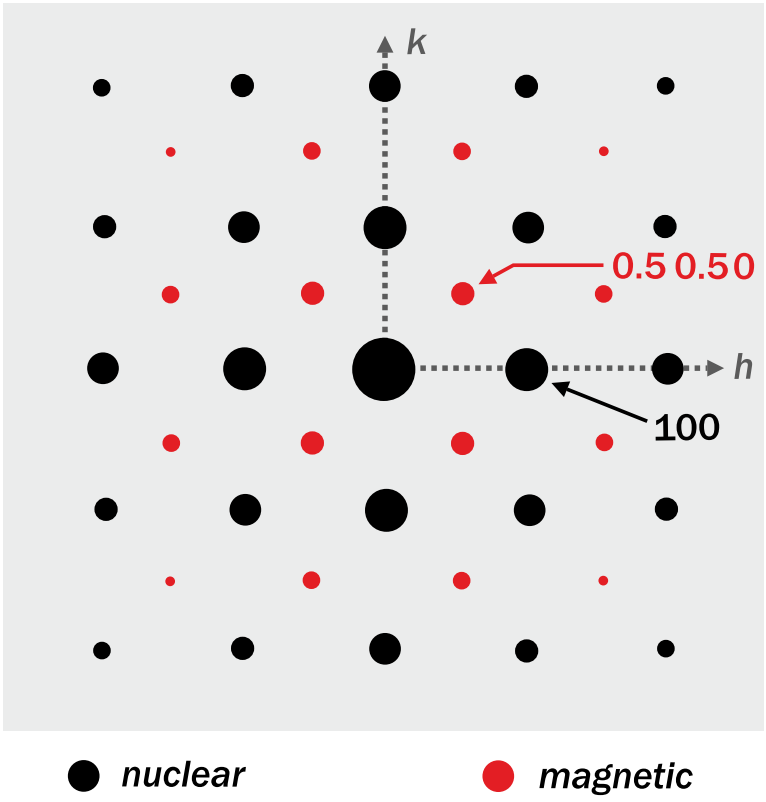
Intensities of reflections $\longrightarrow$ **atomic positions**

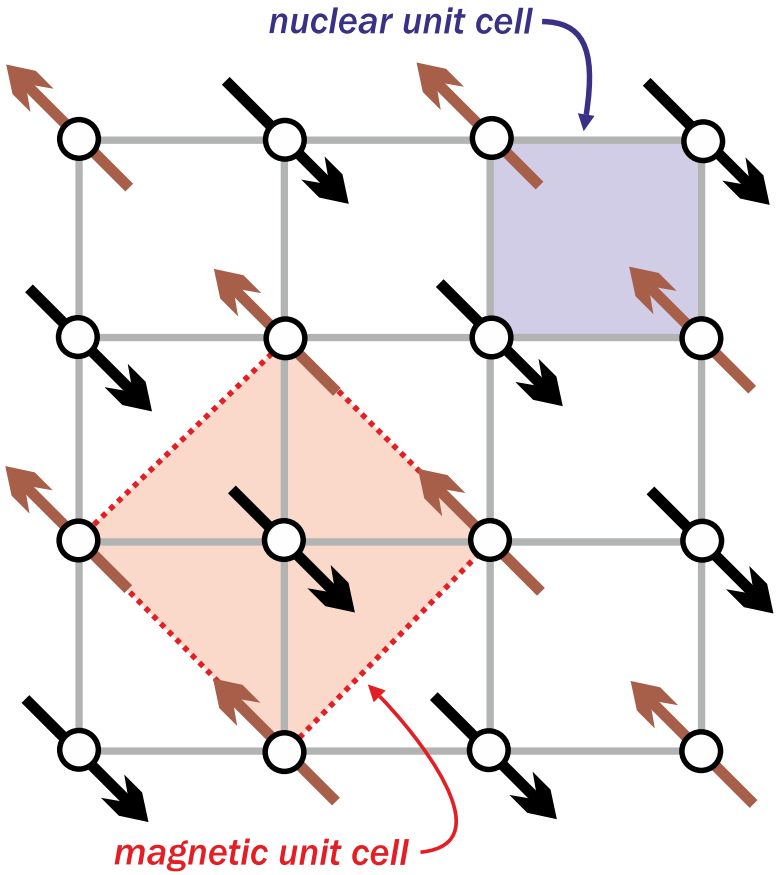
Image credit: LibreTexts Chemistry (CC-BY-SA)



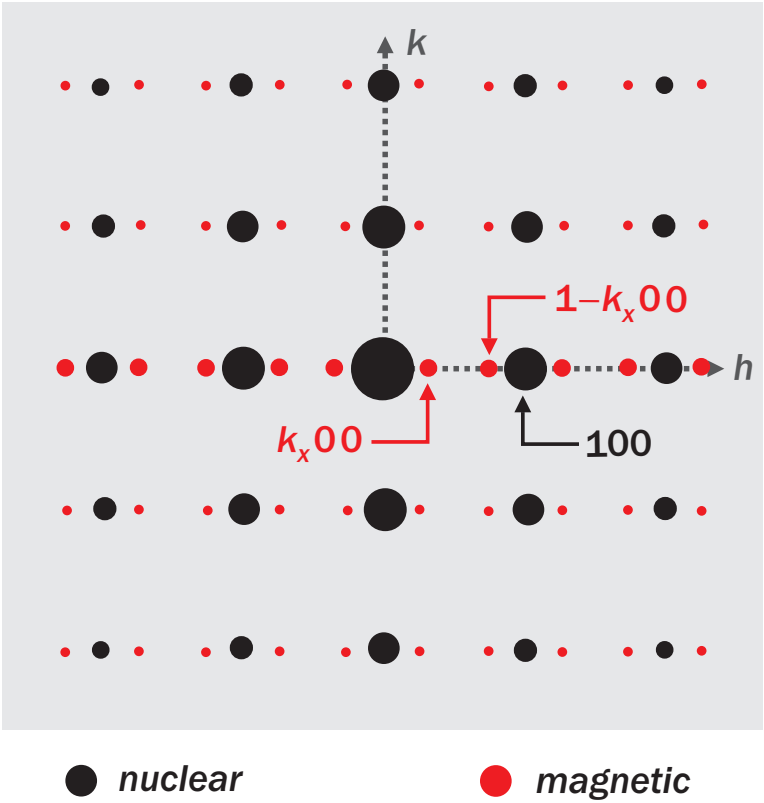


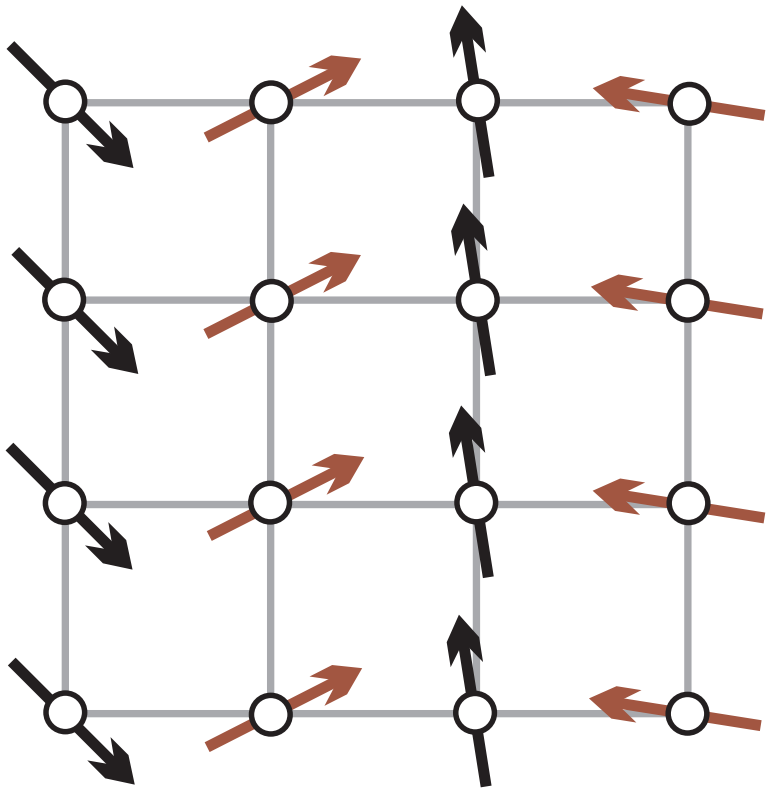
Stripe antiferromagnetic order: $\mathbf{k} = (\frac{1}{2}, 0, 0)$



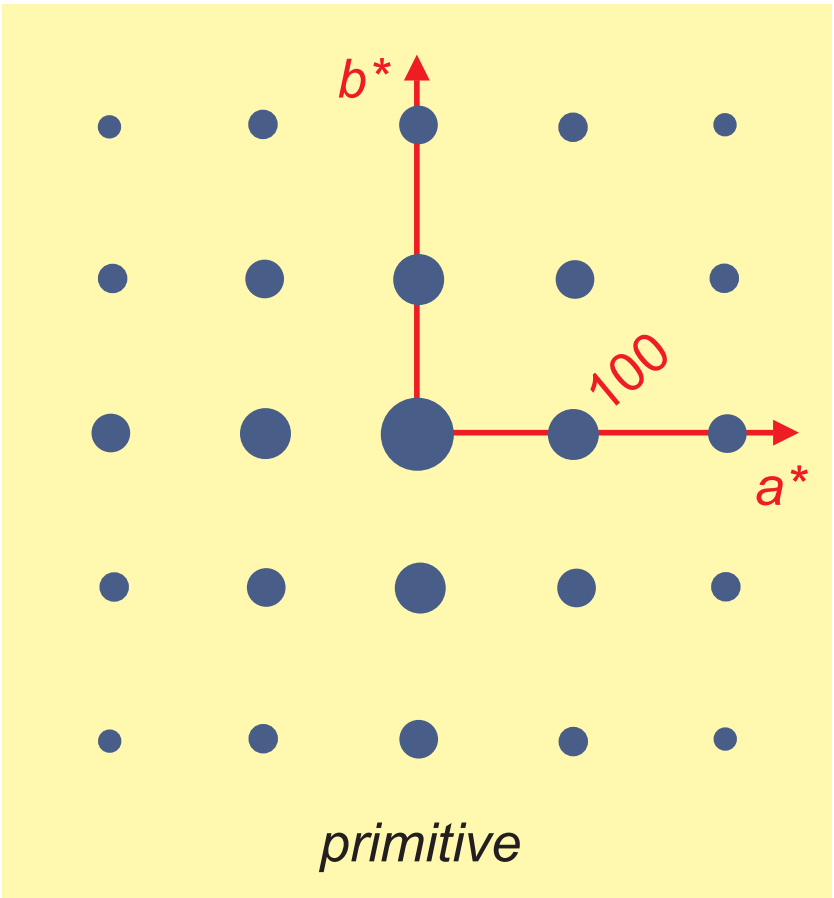


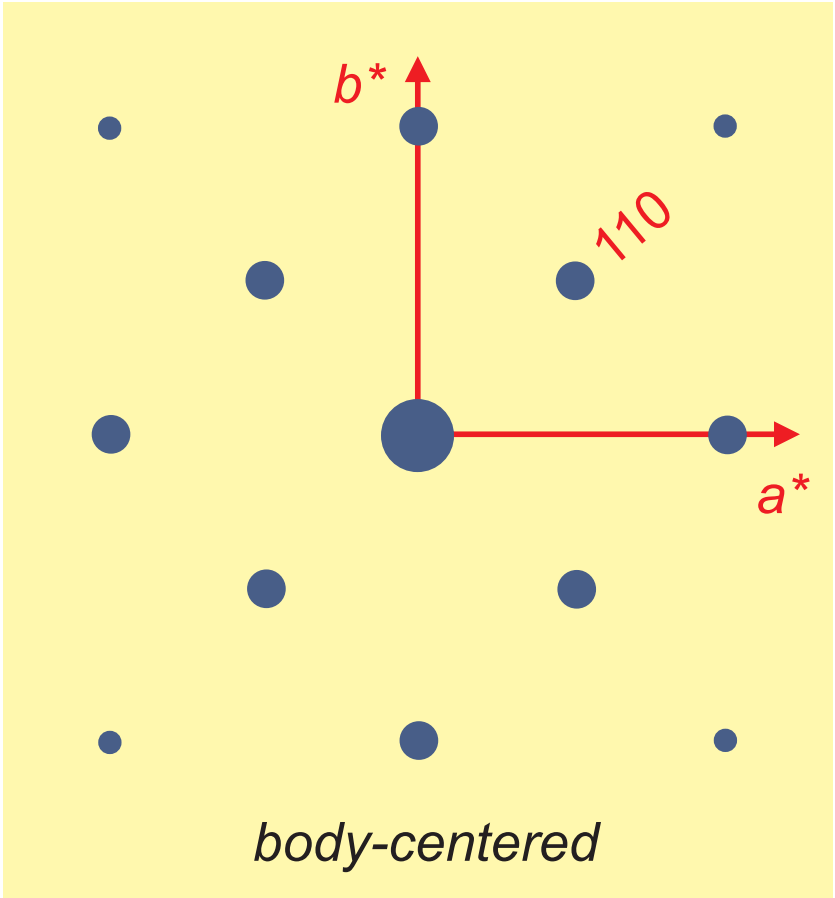
"Standard" (Néel) antiferromagnetic order: $\mathbf{k} = (\frac{1}{2}, \frac{1}{2}, 0)$

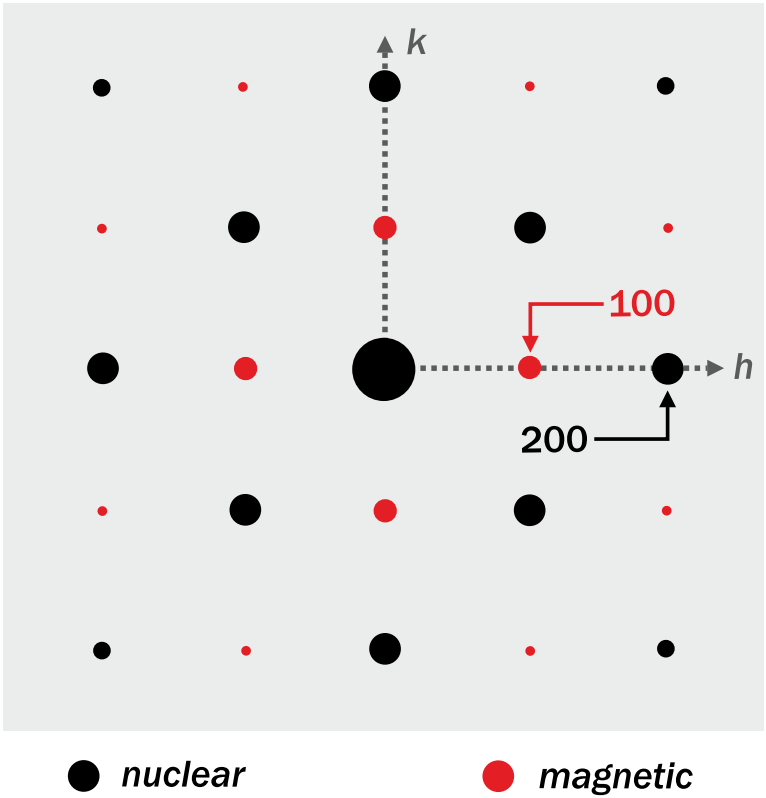


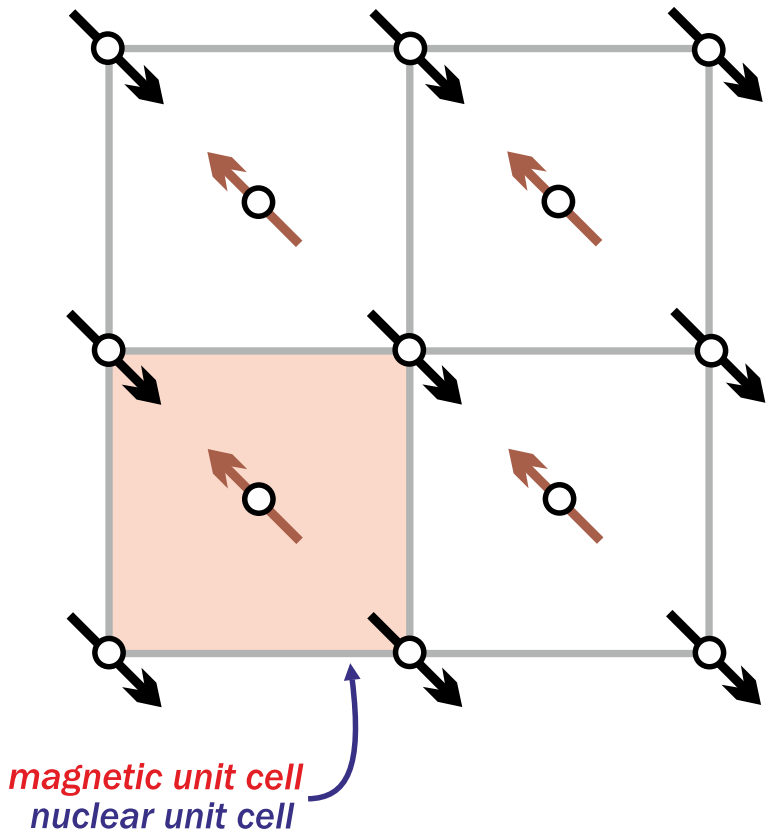


Incommensurate magnetic order: $\mathbf{k} = (0.21456, 0, 0)$

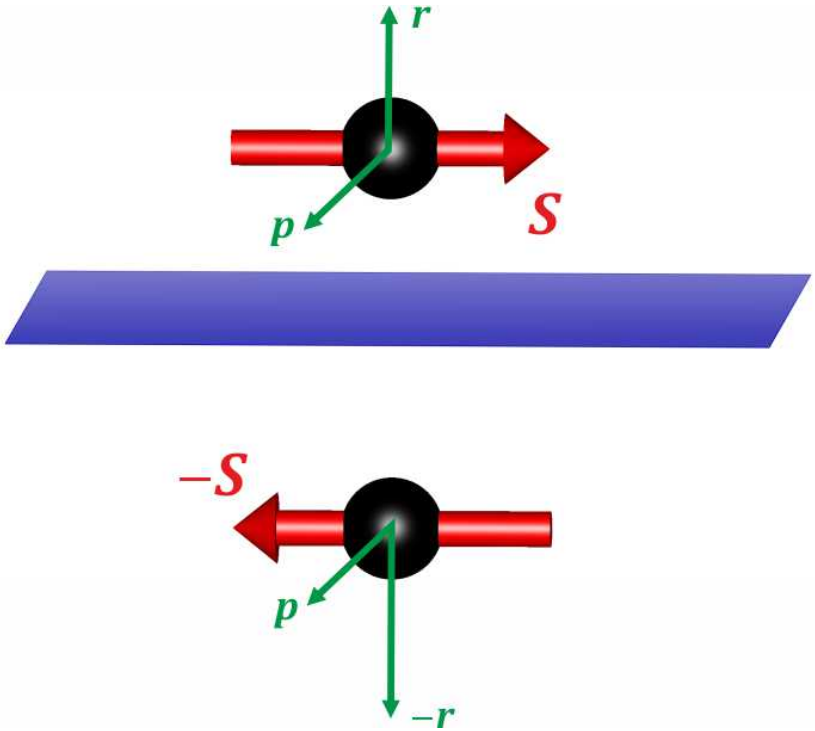

b*
100
a*
primitive

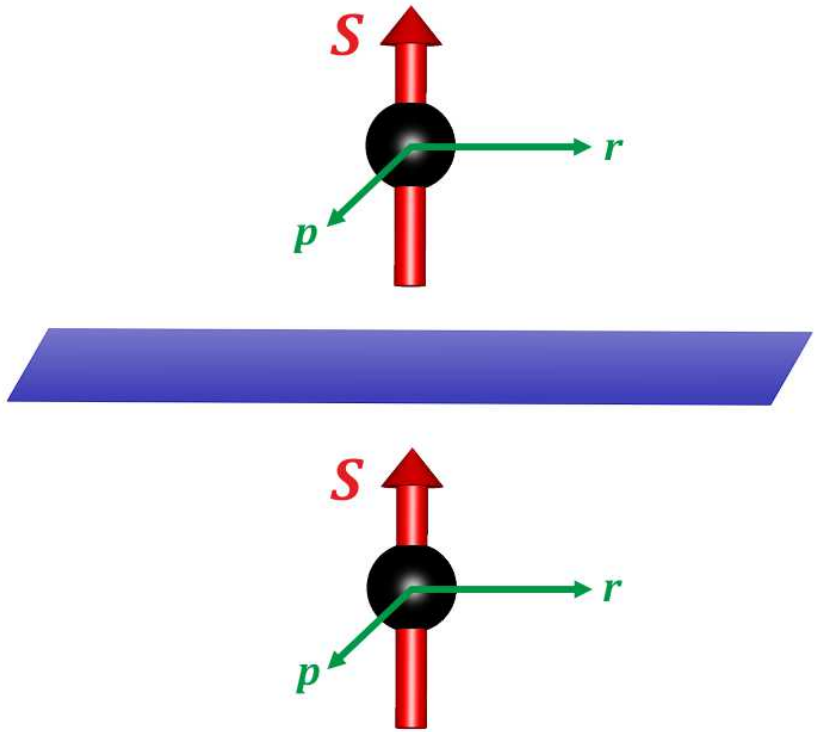

b*
110
a*
body-centered





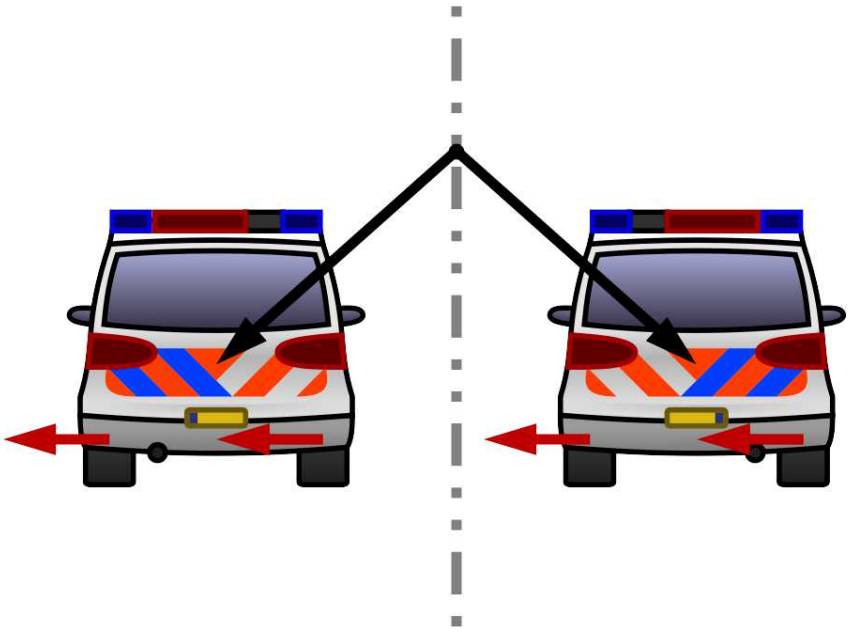
Body-centered lattice: $\mathbf{k} = (1, 0, 0)$

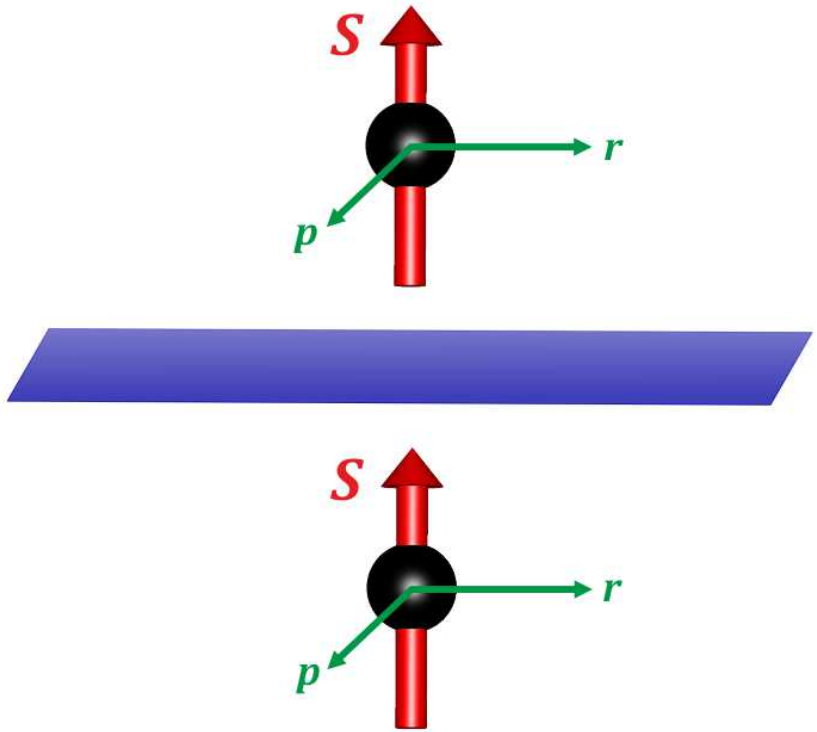




Spin is an **axial vector** (pseudovector)!

Image credit: Gerbrant (CC-BY-SA)





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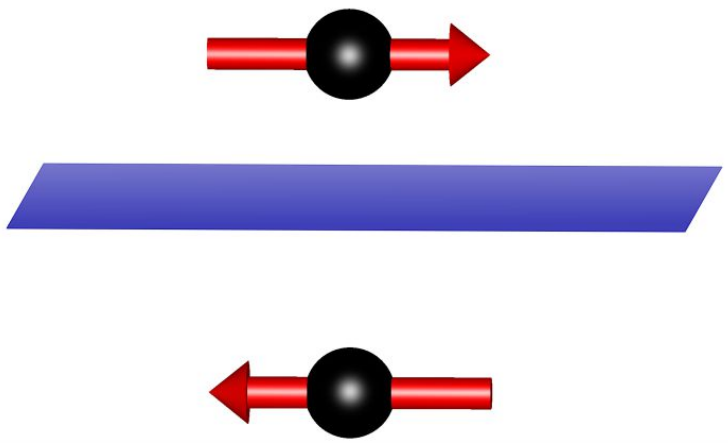
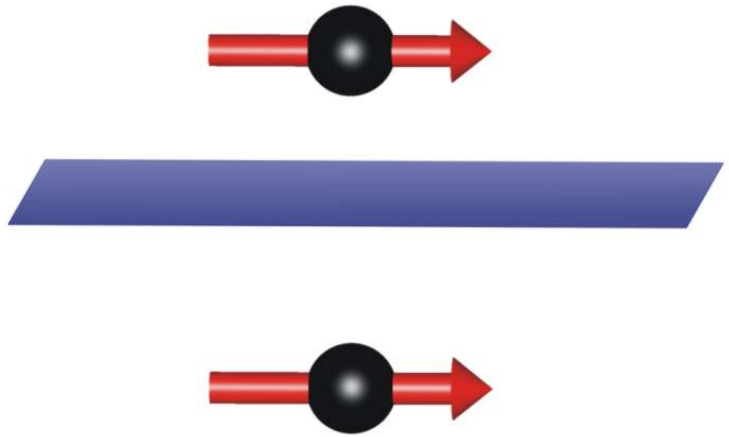
Symmetry elements + spin flip

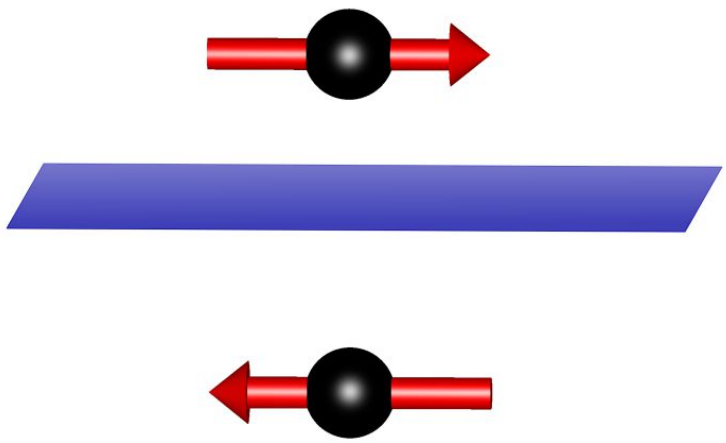


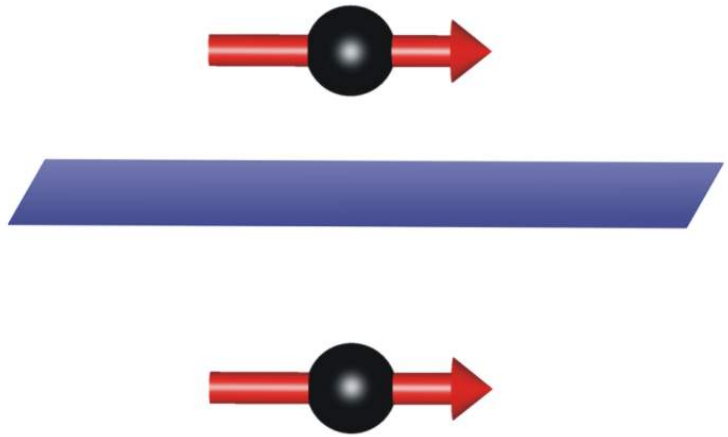
m = reflection in the mirror plane



m' = reflection + spin flip

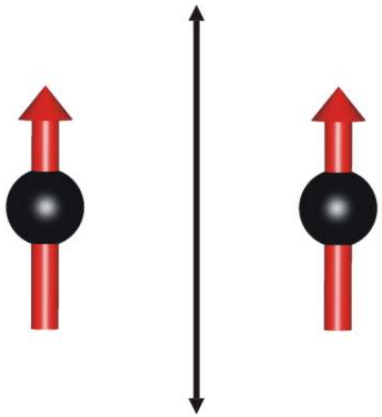
Symmetry elements + spin flip





m = reflection in the mirror plane

m' = reflection + spin flip



2 =

two-fold

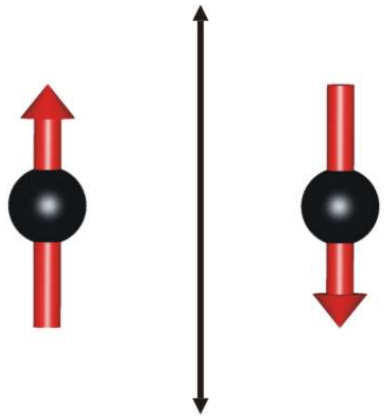
rotation

$2'$ =

rotation

+

spin flip



Black-and-white point groups

$4'm'm$

Black-and-white point groups

$4'm'm$

$4'mm'$

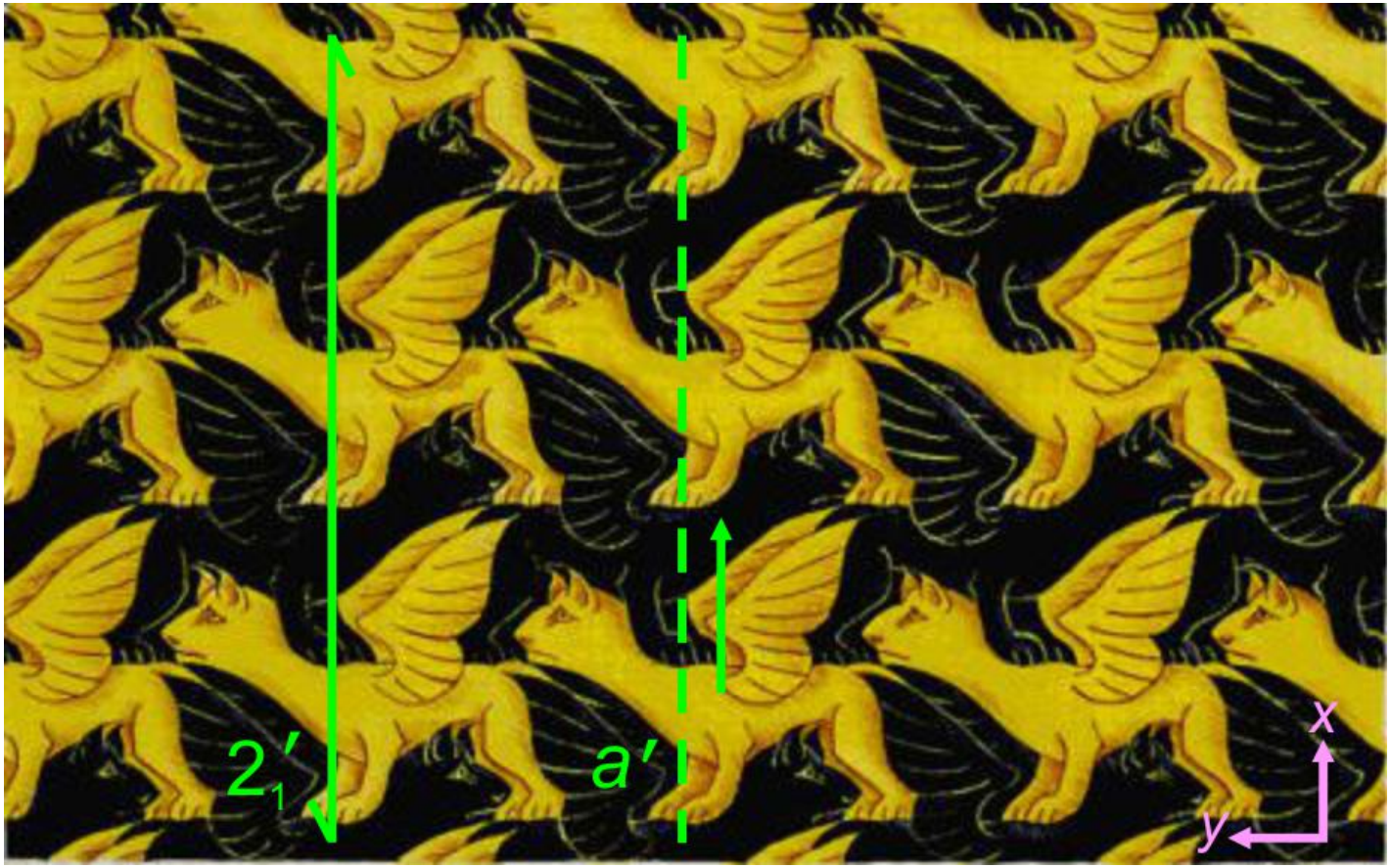
Black-and-white point groups

$4'm'm$

$4'mm'$

$4m'm'$

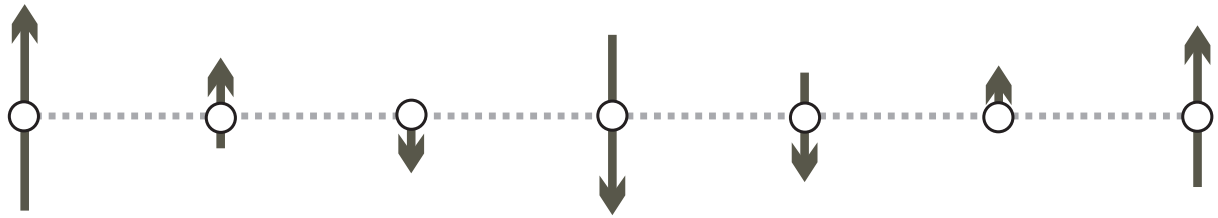
M.C. Escher. Winged lion



M.C. Escher. Winged lion

Black-and-white (Shubnikov) group: $P\,2'_1 a' m$

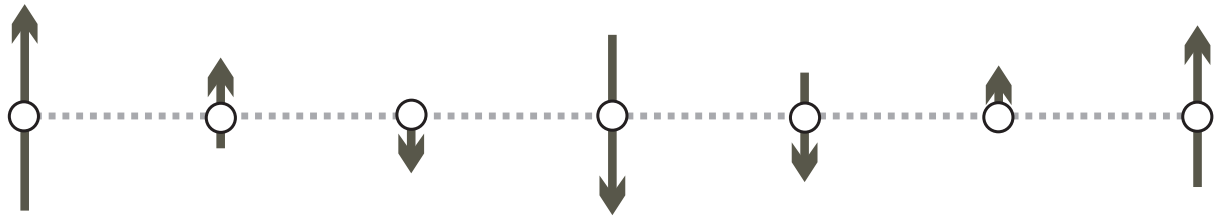
Types of incommensurate magnets



Spin-density wave

$$\mathbf{S} = \mathbf{S}_0 \cos qa$$

Types of incommensurate magnets



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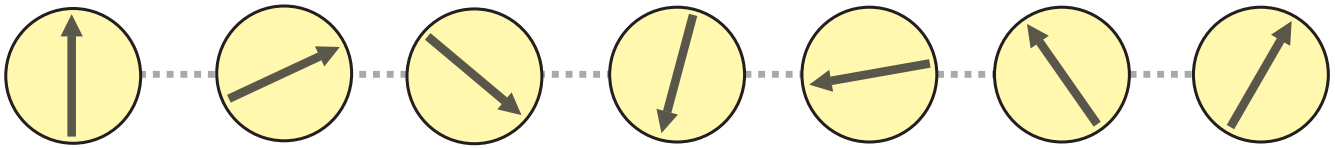
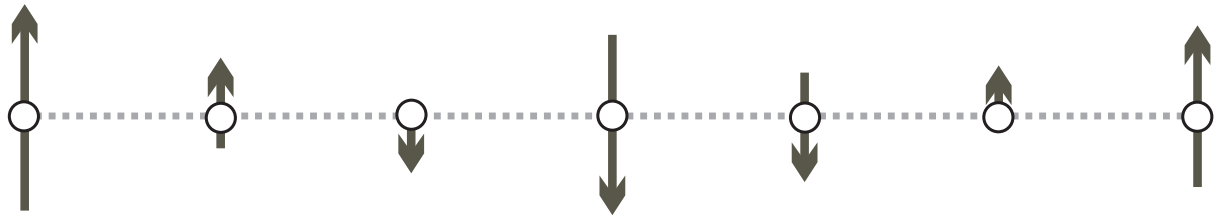


Cycloid

$$S^x = S_0\, e^{iqa}$$
$$S^y = iS^x,\ S^z = 0$$

$$\mathbf{k} = (0, k_y, 0)$$

Types of incommensurate magnets



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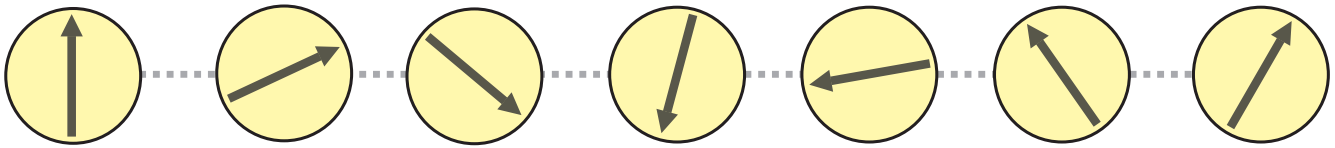

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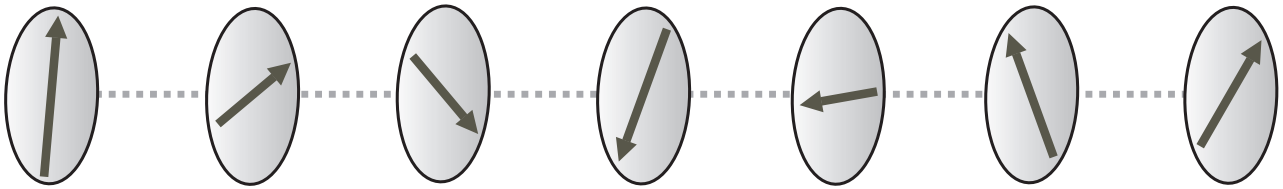


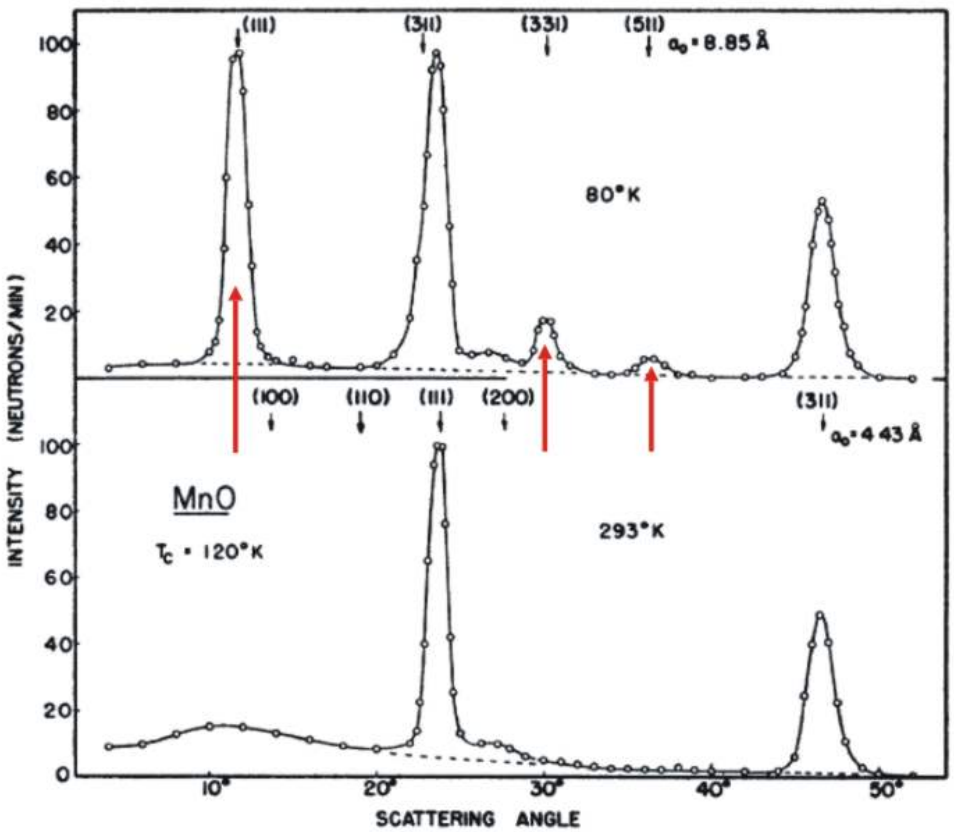
Helix

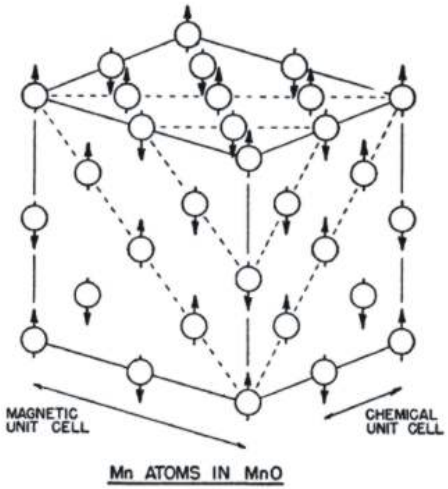
$$S^x = S_0\, e^{iqa}$$
$$S^z = iS^x,\ S^y = 0$$
$$\mathbf{k} = (0, k_y, 0)$$

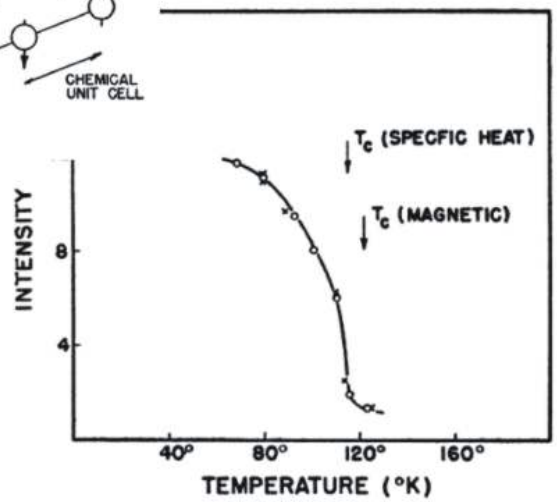
Experiment

neutron diffraction

Proof of antiferromagnetism





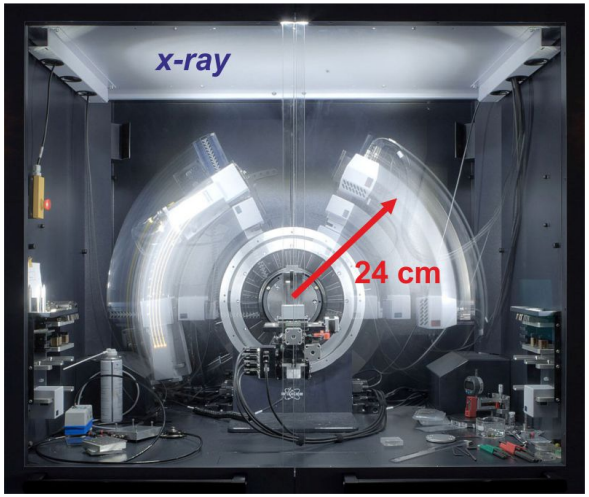


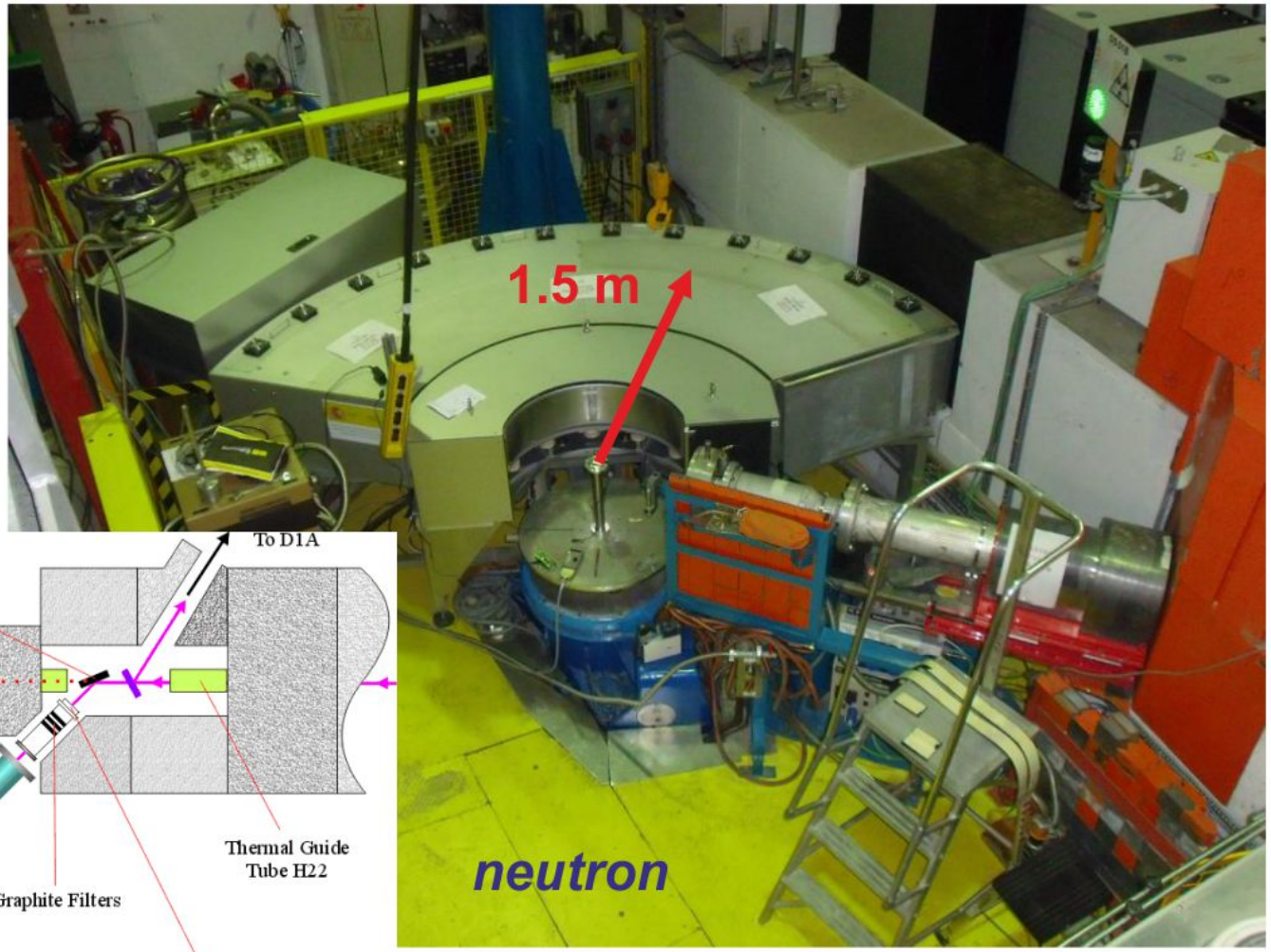
Magnetic order $\longrightarrow$ additional periodicity

$\longrightarrow$ additional peaks in neutron diffraction

Phys. Rev. 76, 1256 (1949) and Phys. Rev. 83, 333 (1951)

Neutron diffractometer





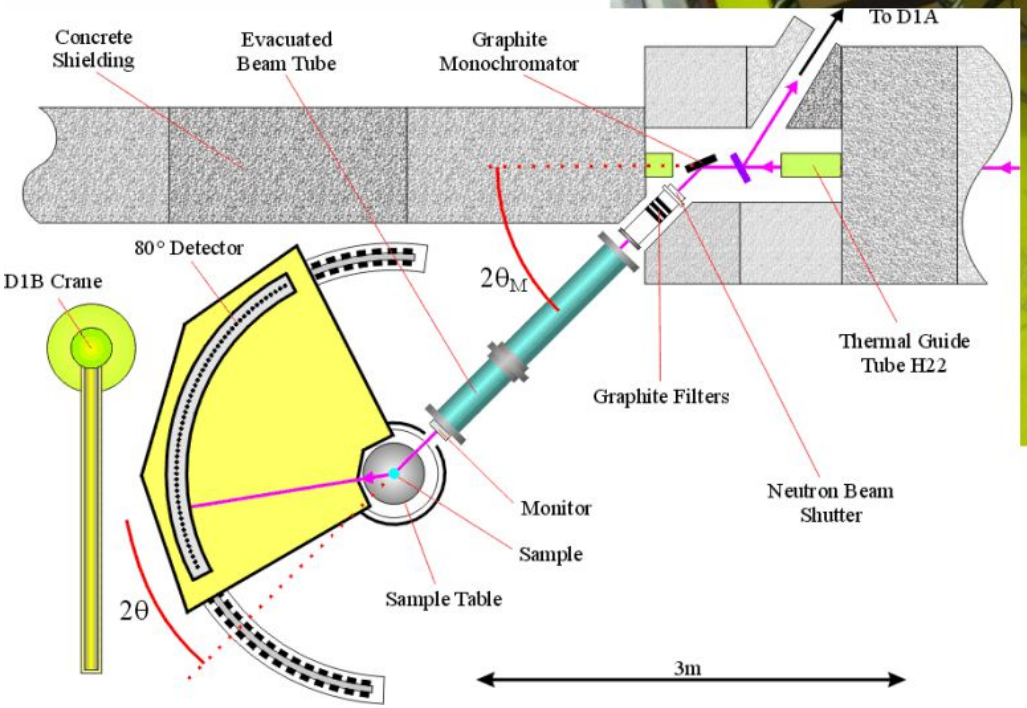


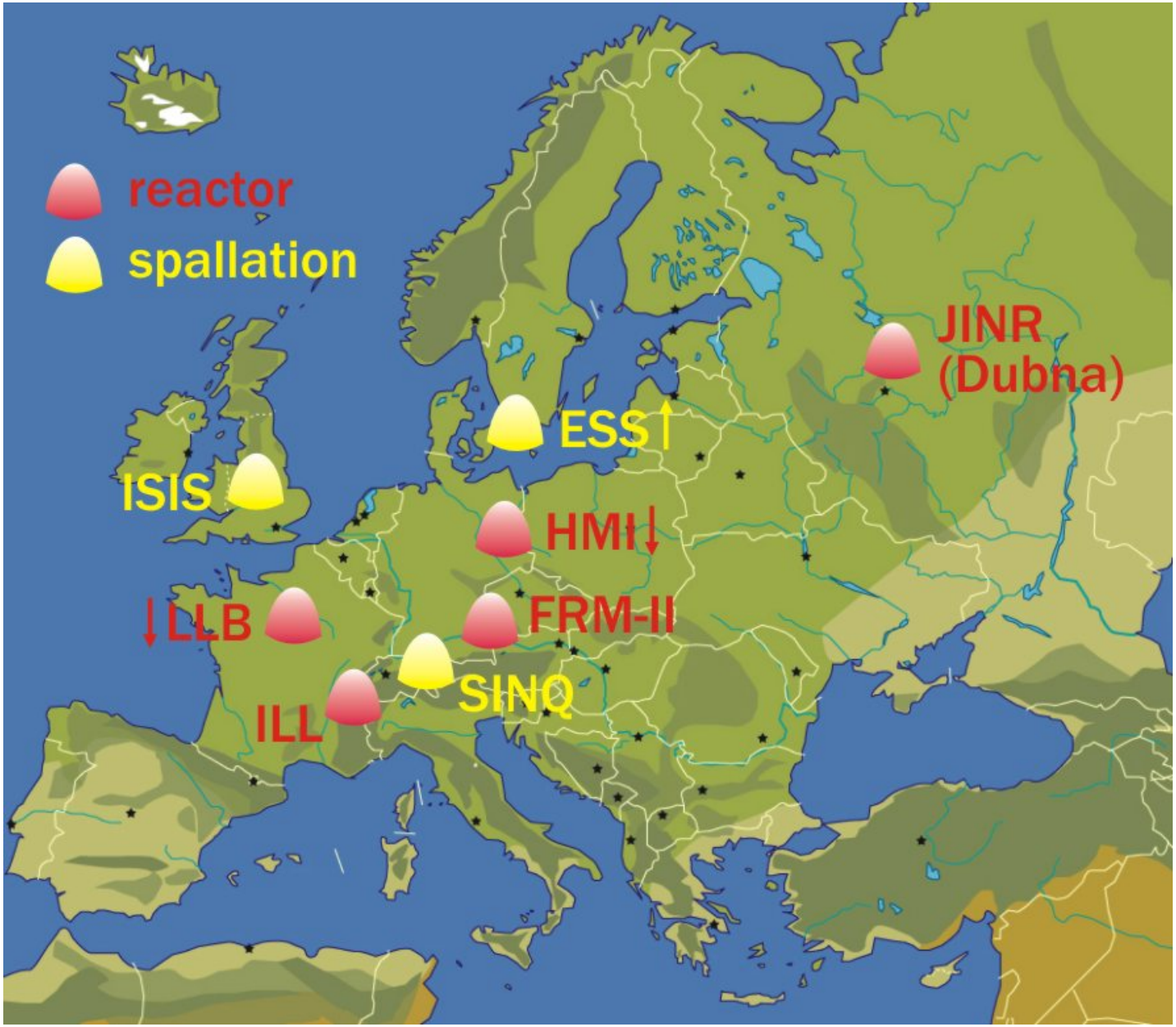
Image credits:
Kaspar Kallip (CC-BY-SA)
J. Phys. Conference Series 549, 012003 (2014)
Birkbeck College, UCL

- **Nuclear reactor:**
  stable and robust neutron source,
  but requires huge infrastructure
  + environmental concerns

- **Spallation source:**
  neutrons may arrive in pulses
  less stable in general,
  but more environment-friendly,
  and higher flux can be achieved

Image credits: Andreas Battenberg / TUM (fair use) and U.S. Department of Energy (public domain)

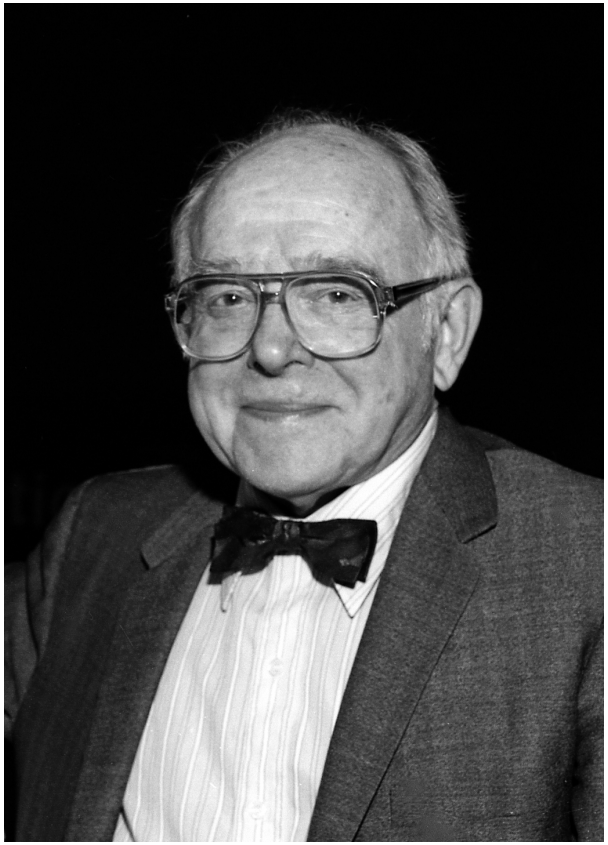
Neutron sources in Europe



Map source: Johomaps

Person

Clifford Shull

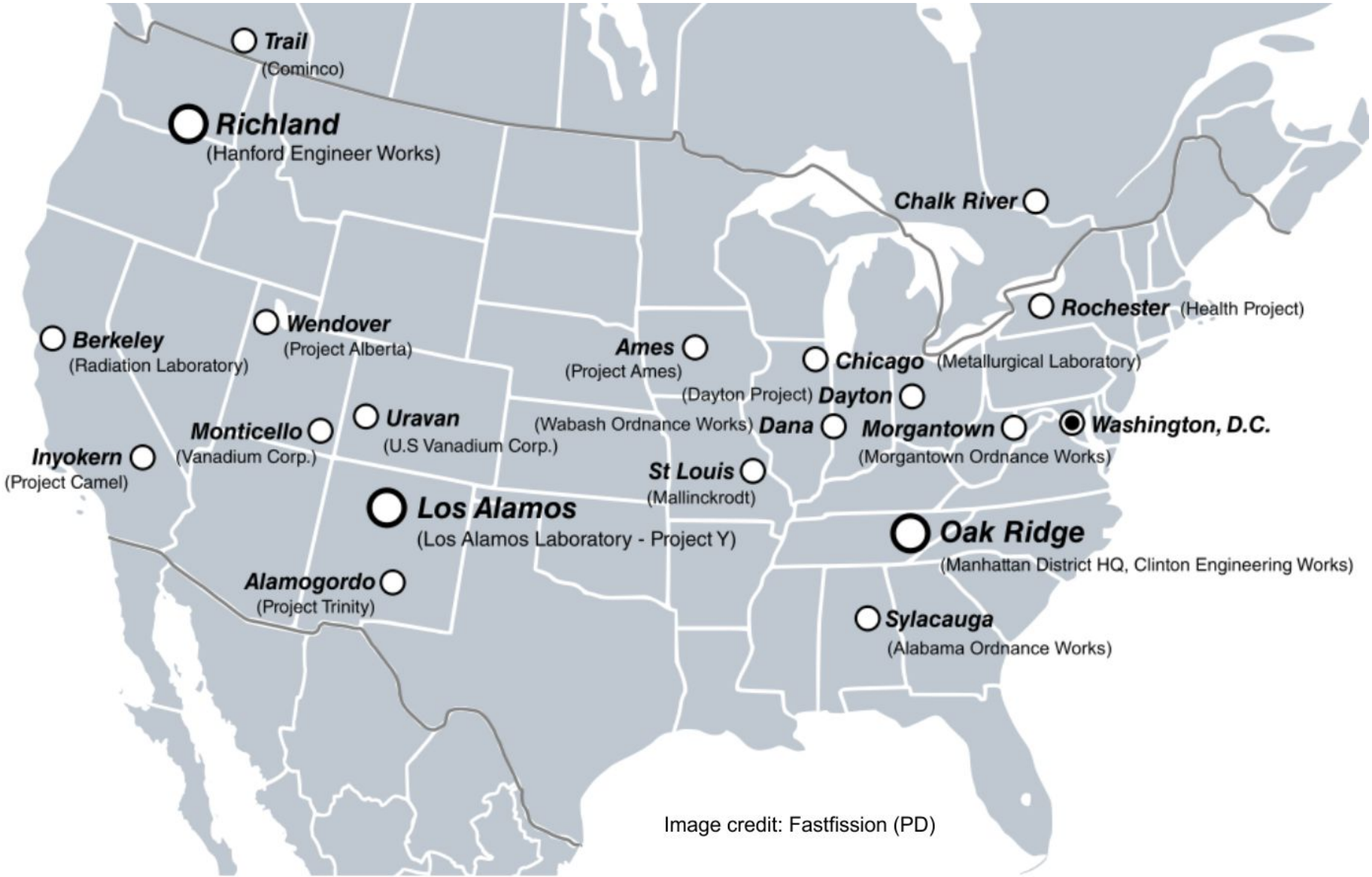


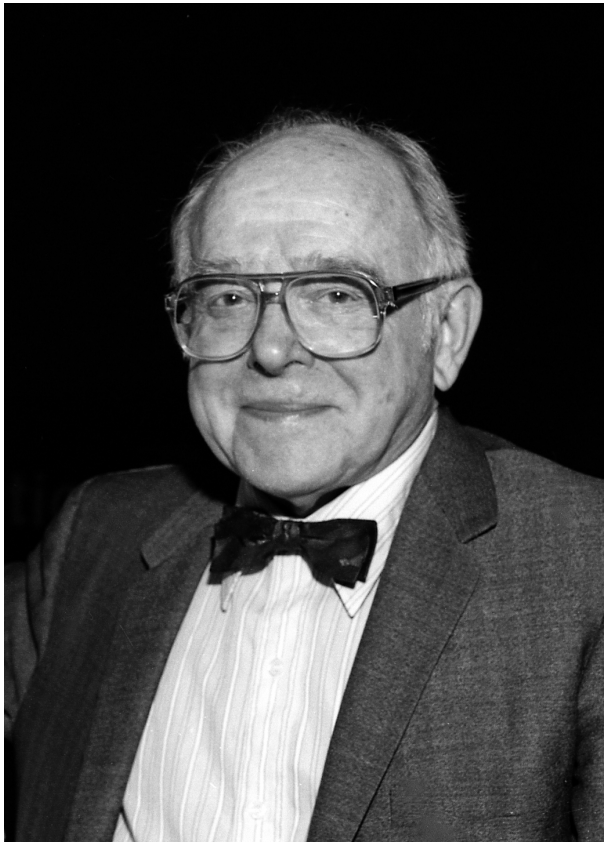
Clifford Shull

1915–2001

- 1937: Physics studies at Carnegie Institute of Technology, Pittsburg
- 1941: PhD in physics, New York University
- 1941–1946: work at Texas Company, development of aviation fuels and lubricants

Manhattan Project





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  - positions of light atoms (1948)
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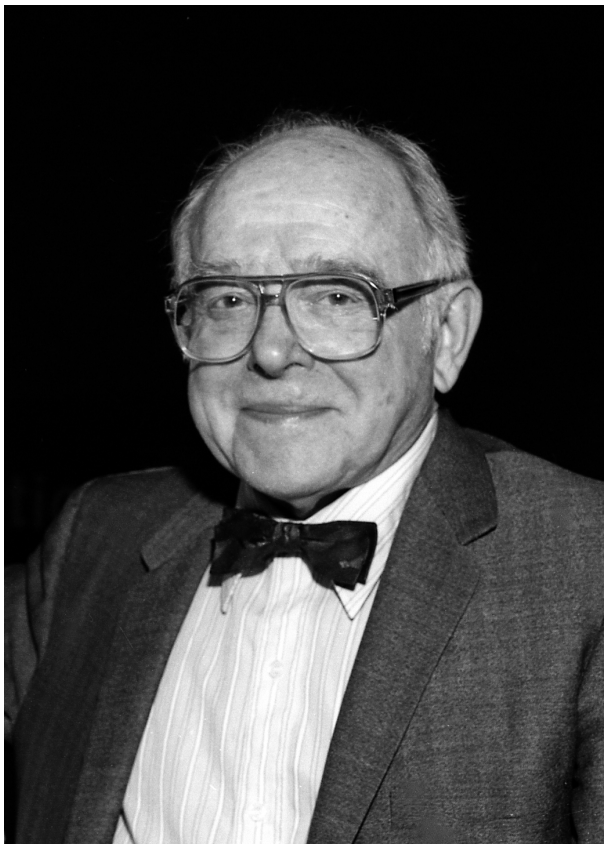

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