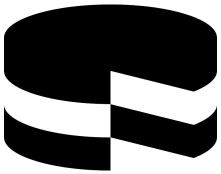
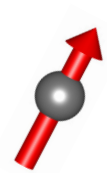
Structure factor: All shades of diffraction

neutron diffraction



solid hydrogen

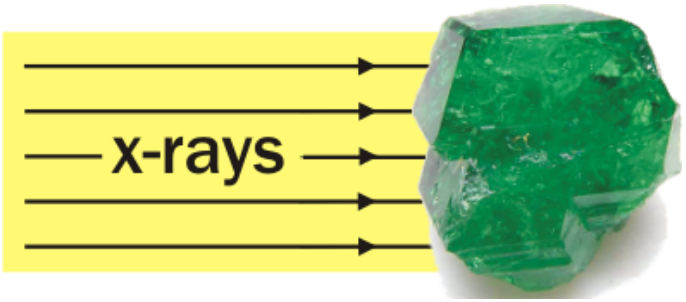
DNA team

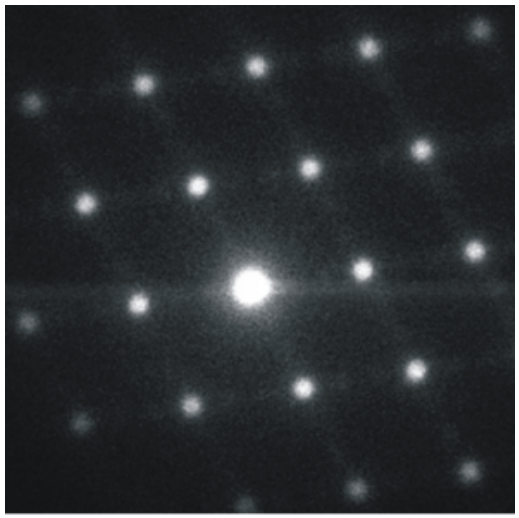


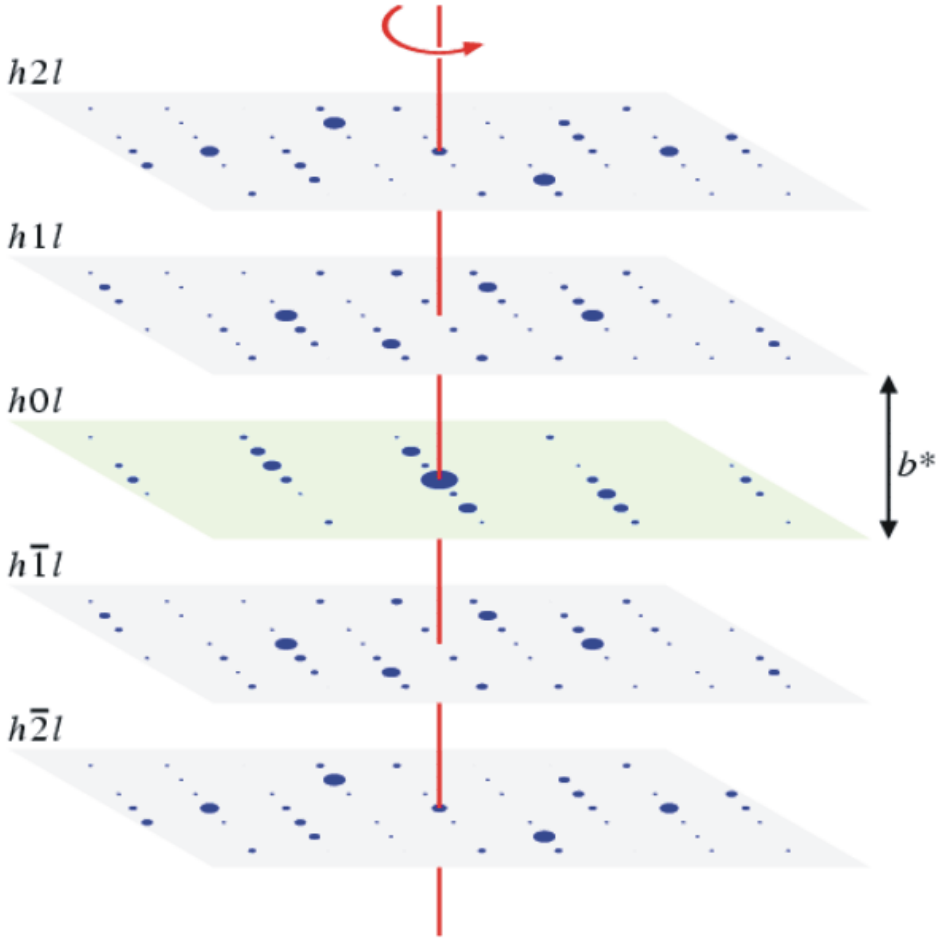
by Alexander Tsirlin, Leipzig University

Lecture 6: October 26, 2023

Diffraction from single crystals

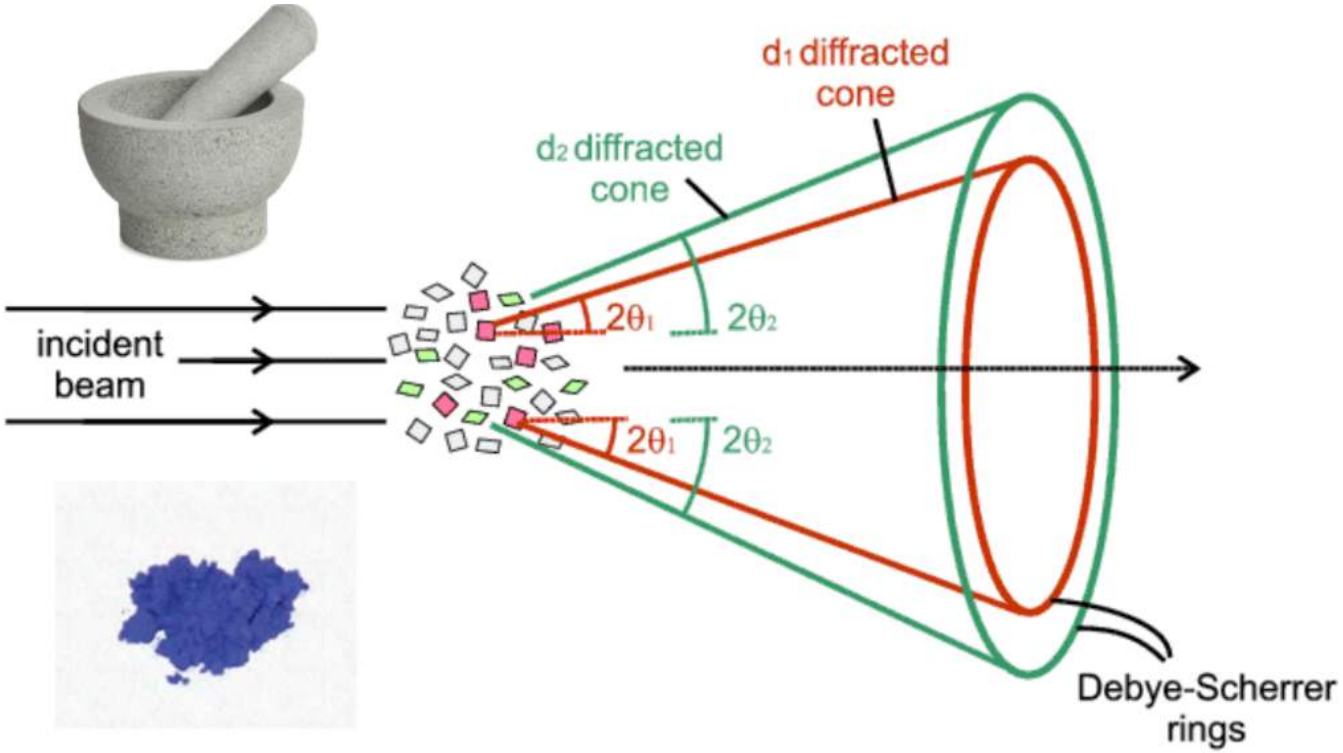


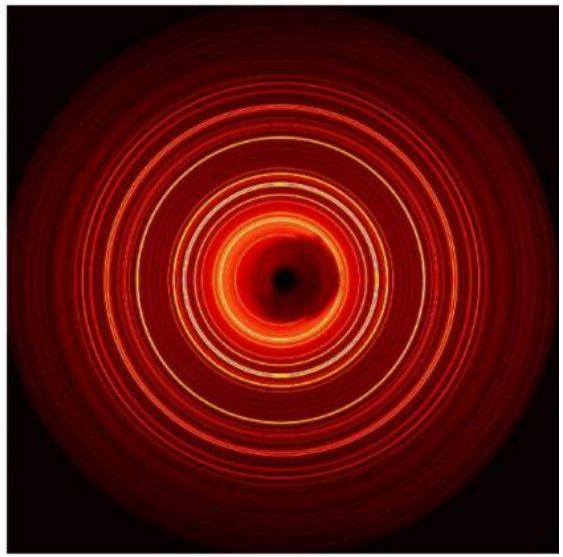




Diffraction pattern is an image of the reciprocal lattice

Diffraction from powders

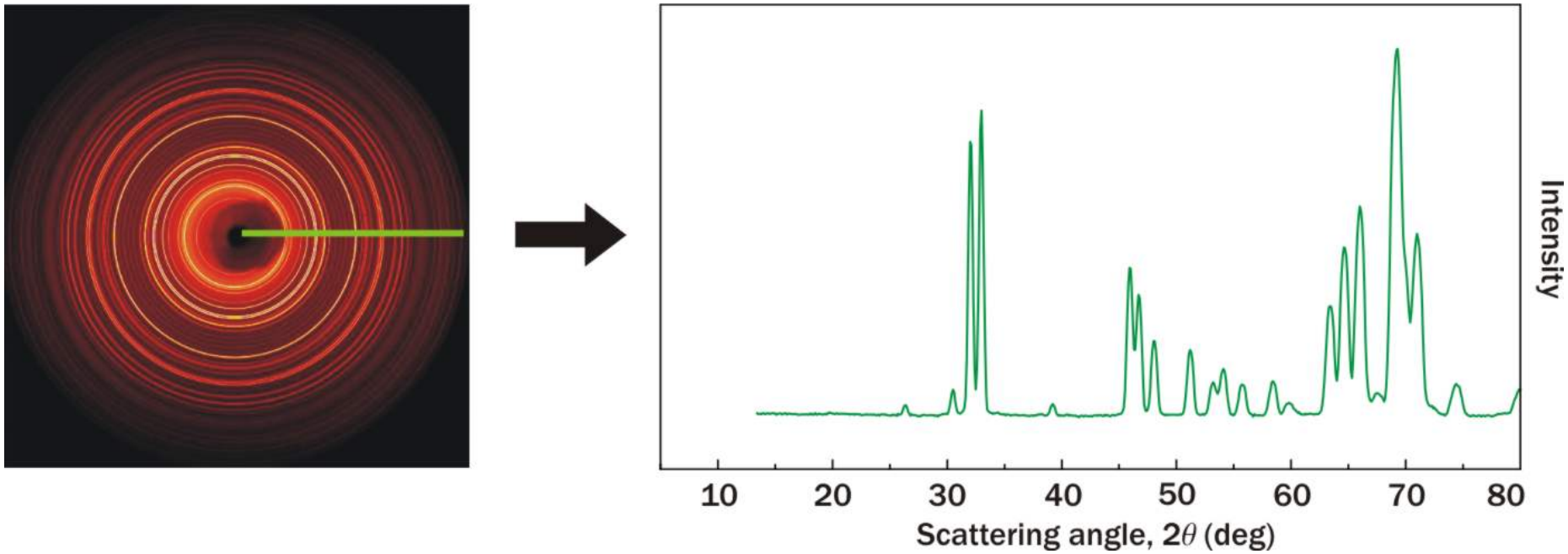




Debye-Scherrer rings, imprints of cones of scattered intensity

Image credit: School of Crystallography, Birkbeck College, University of London

Diffraction from powders

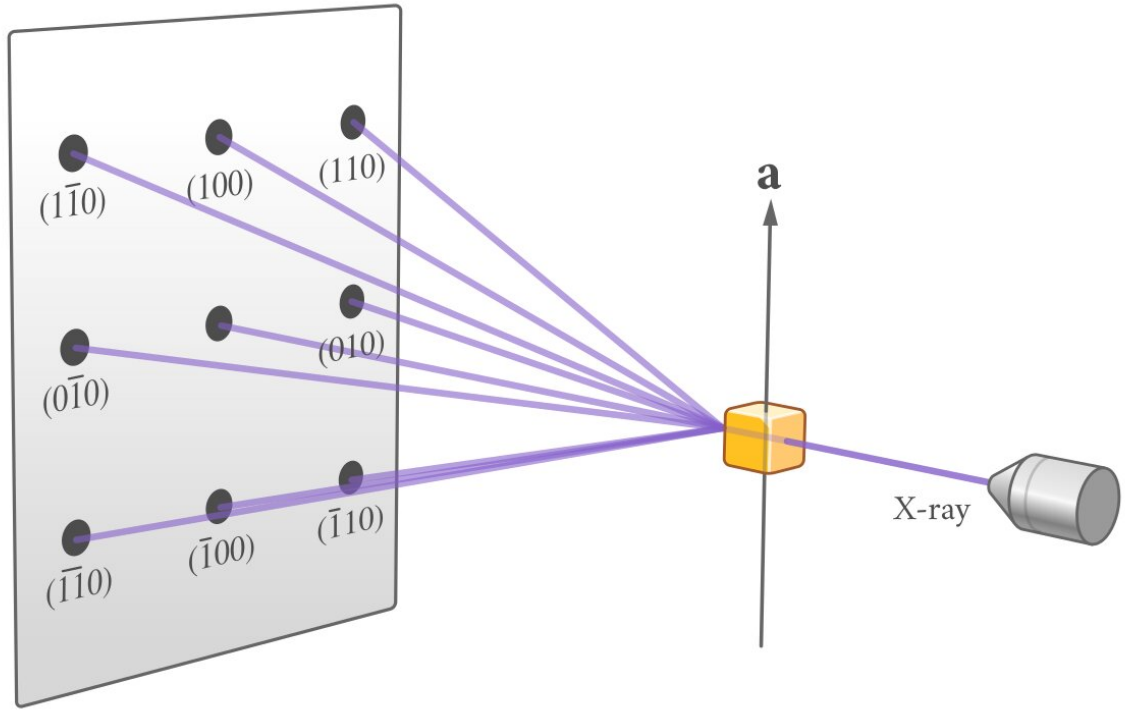


Debye-Scherrer rings, imprints of cones of scattered intensity

Single-crystal: **3D pattern**, powder: **1D pattern**

Image credit: School of Crystallography, Birkbeck College, University of London

“Philosophy” of diffraction experiments



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

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

Body-centered lattice

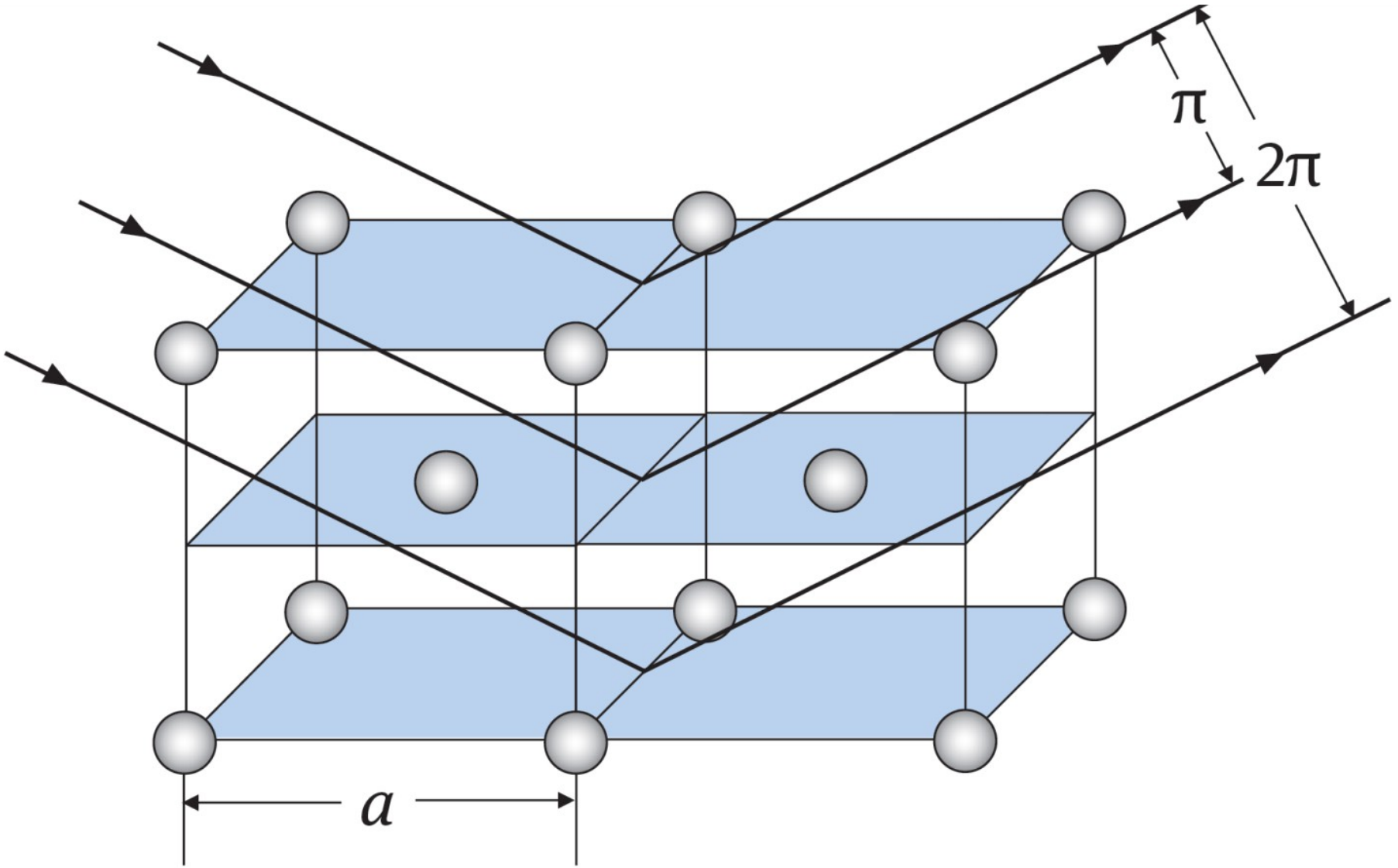
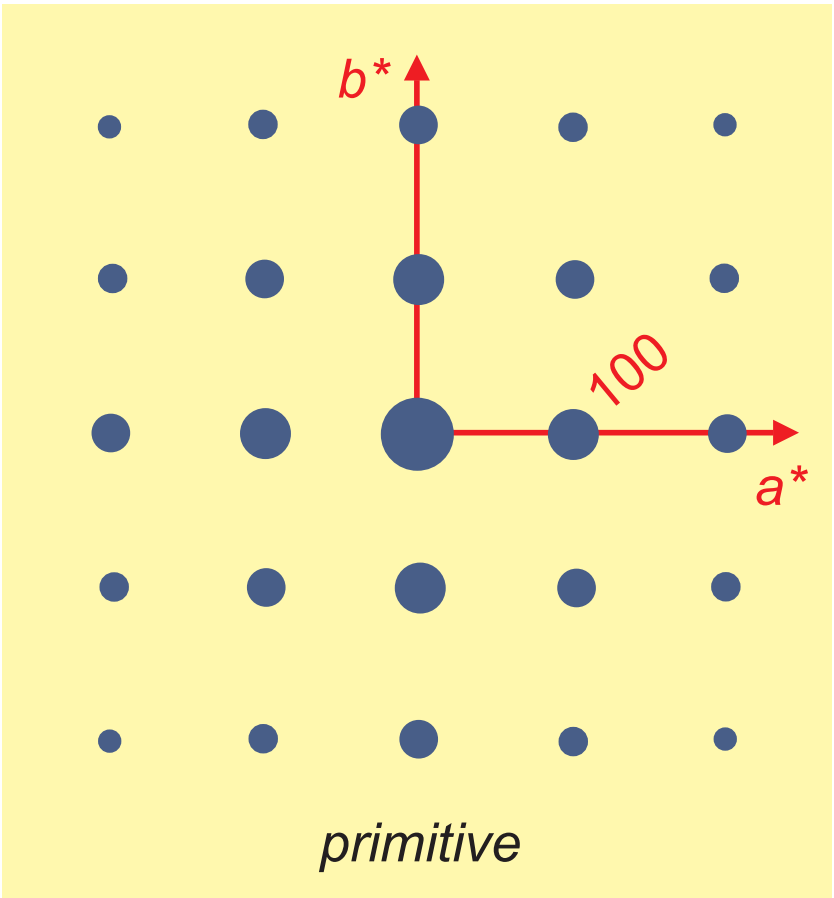
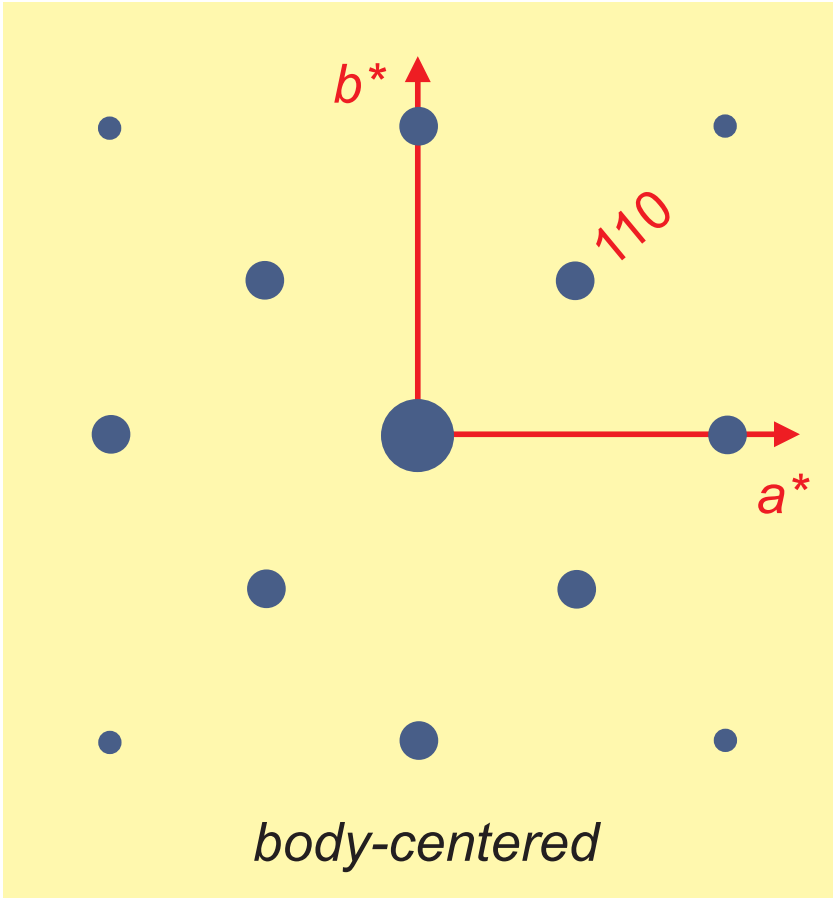


Image credit: Hunklinger, Solid-State Physics

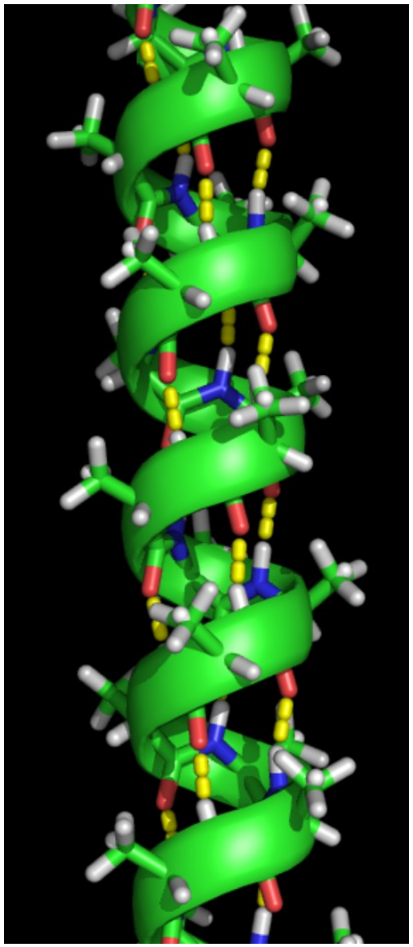

b*
100
a*
primitive


b*
110
a*
body-centered

Person

DNA team

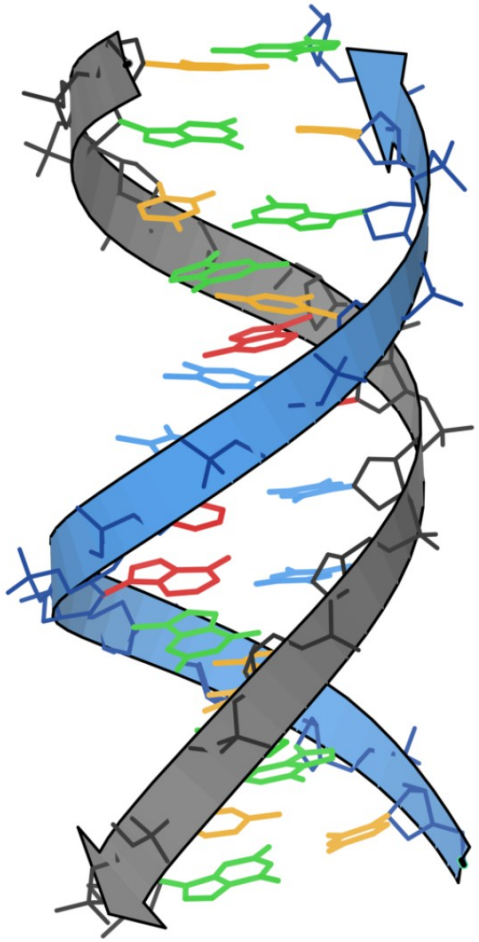
The story of helices



protein

α-helix

(Pauling et al. 1951)



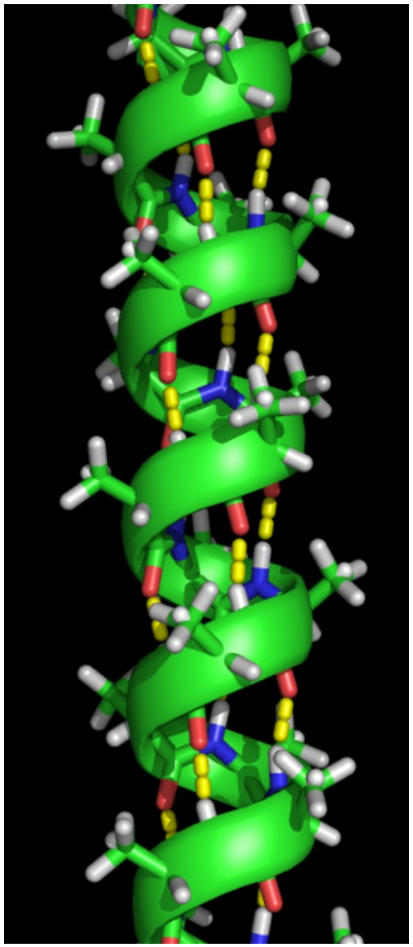
DNA

double helix

1953

Image credit: Dcrjsr and Zsolt Bikadi (CC-BY-SA); Nature 171, 740 (1953)

The story of helices



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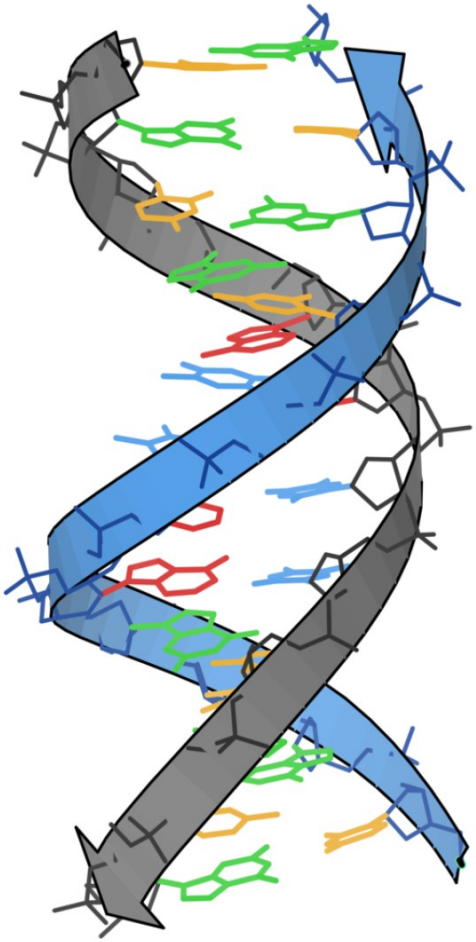
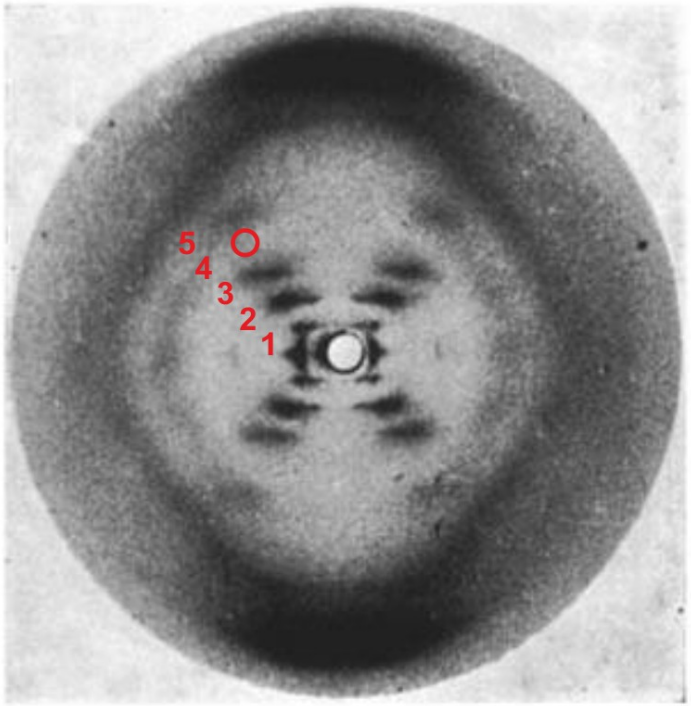


DNA

double helix

1953



diffraction pattern
of DNA (B-form)

Cavendish Laboratory, Cambridge

James Watson
born 1928

Francis Crick
1916–2004

King’s College, London

Maurice Wilkins
1916–2004

Rosalind Franklin
1920–1958

Cavendish Laboratory, Cambridge

James Watson
born 1928

Francis Crick
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1951: first, wrong model of DNA

King's College, London

Maurice Wilkins
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King's College, London

Maurice Wilkins
1916–2004

Rosalind Franklin
1920–1958

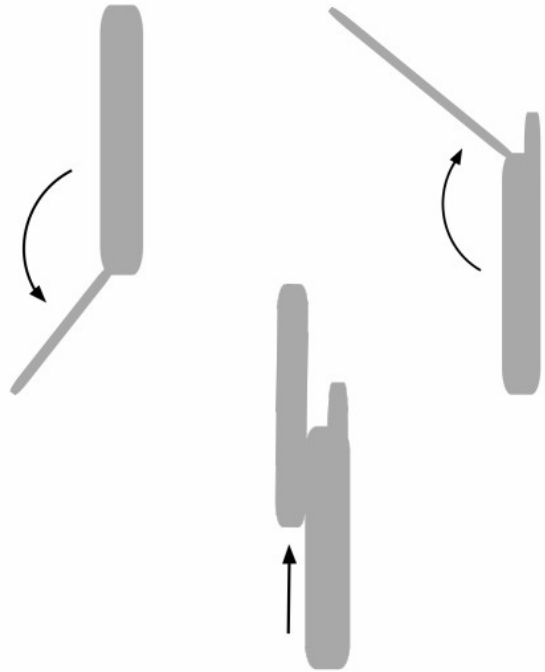
1962 Nobel prize in physiology or medicine: **Watson, Crick, Wilkins**

Experimental technique

neutron diffraction

Form factor (mobile phones)

From Wikipedia, the free encyclopedia



Form factor (mobile phones)

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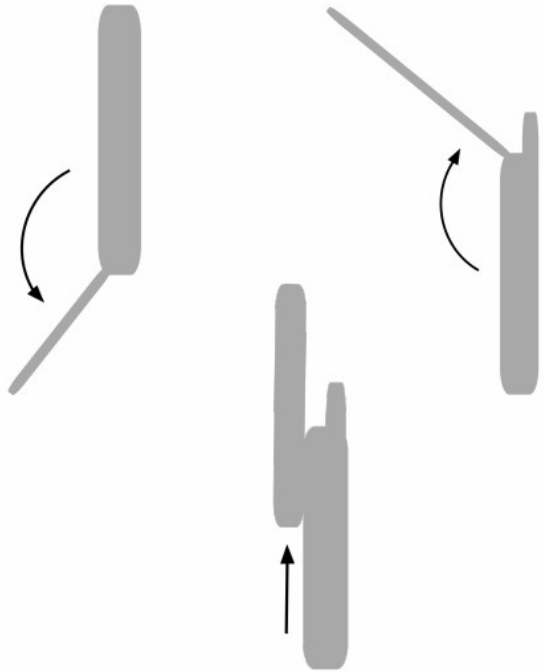
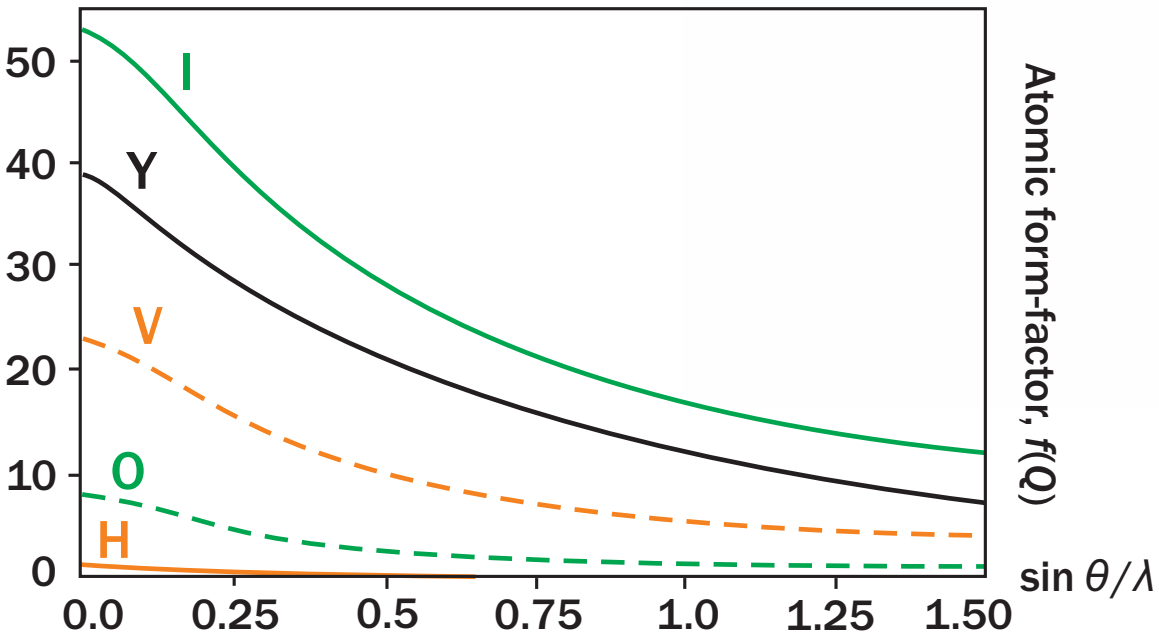
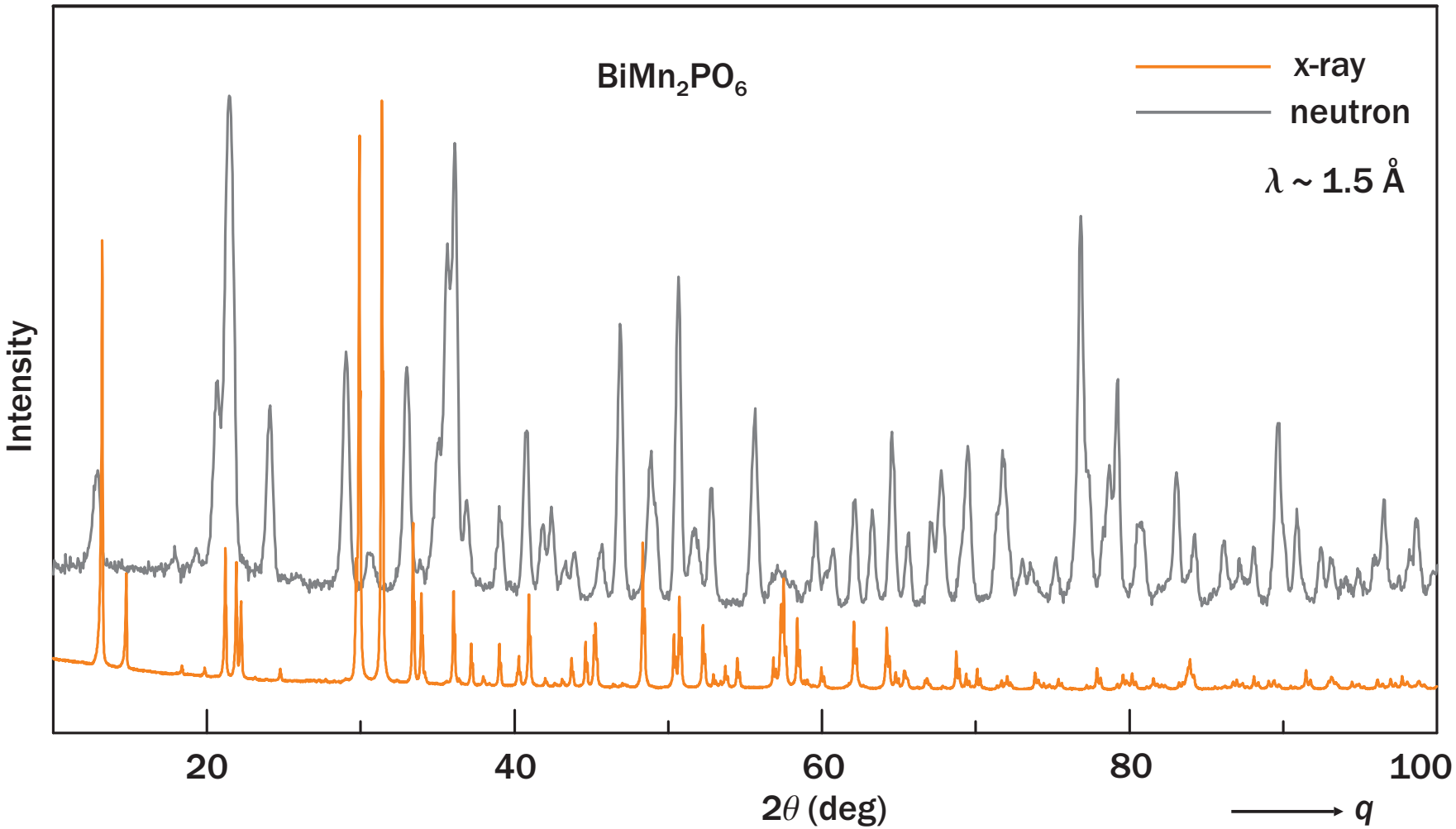


in solid-state physics



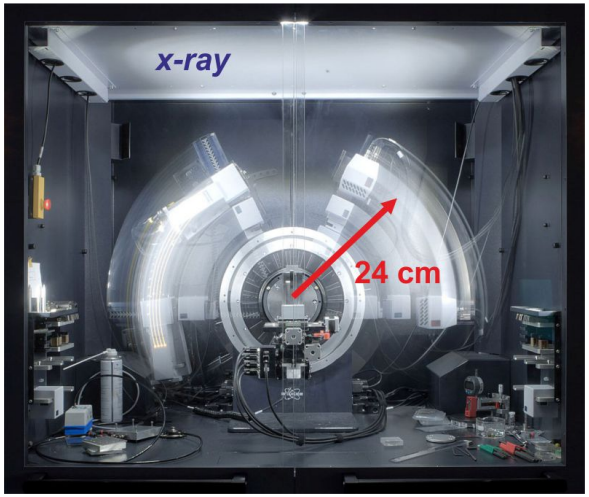
X-ray vs. neutron form-factors

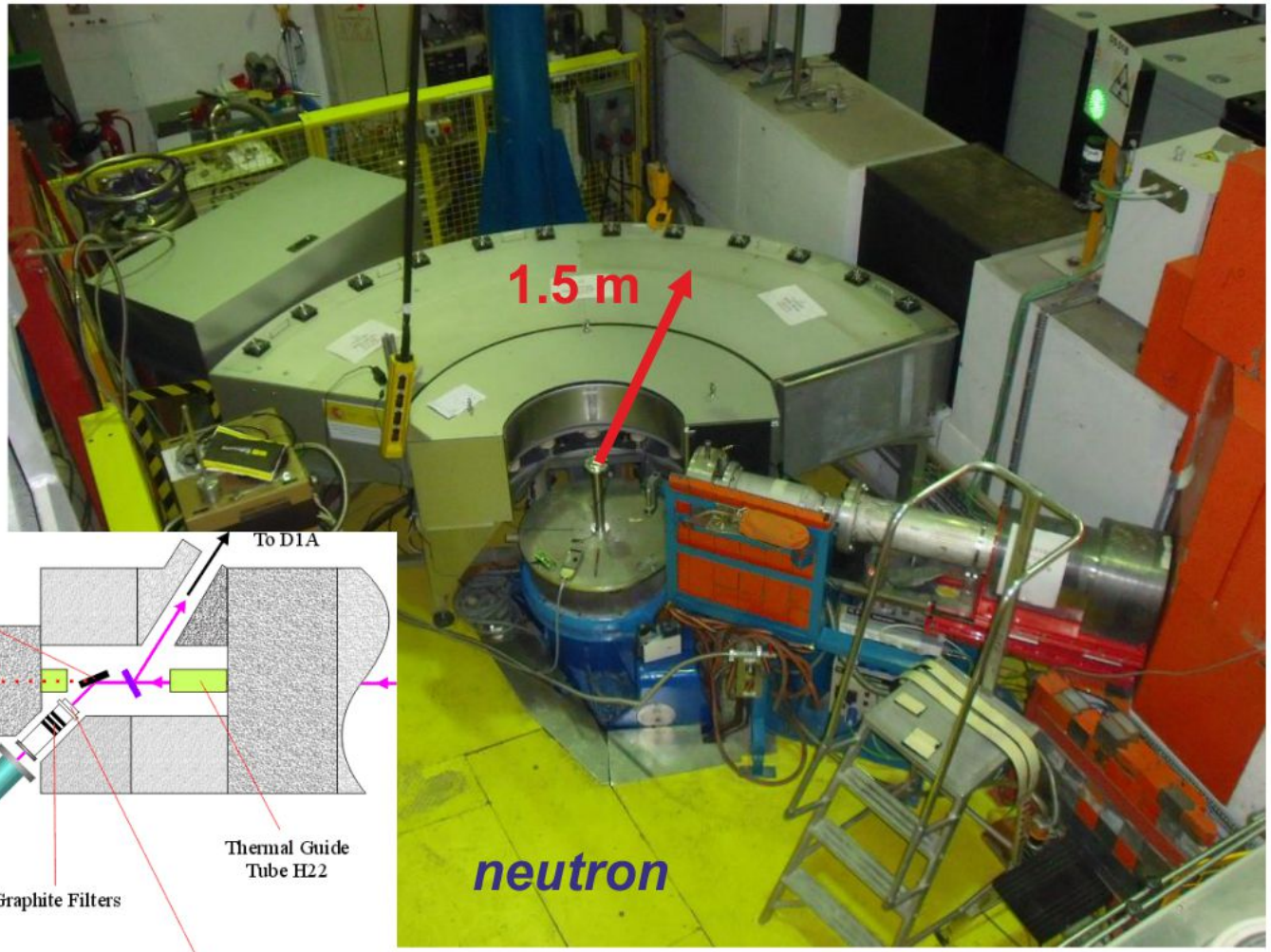


X-ray intensities decrease with q

Neutron intensities are generally q-independent

Neutron diffractometer





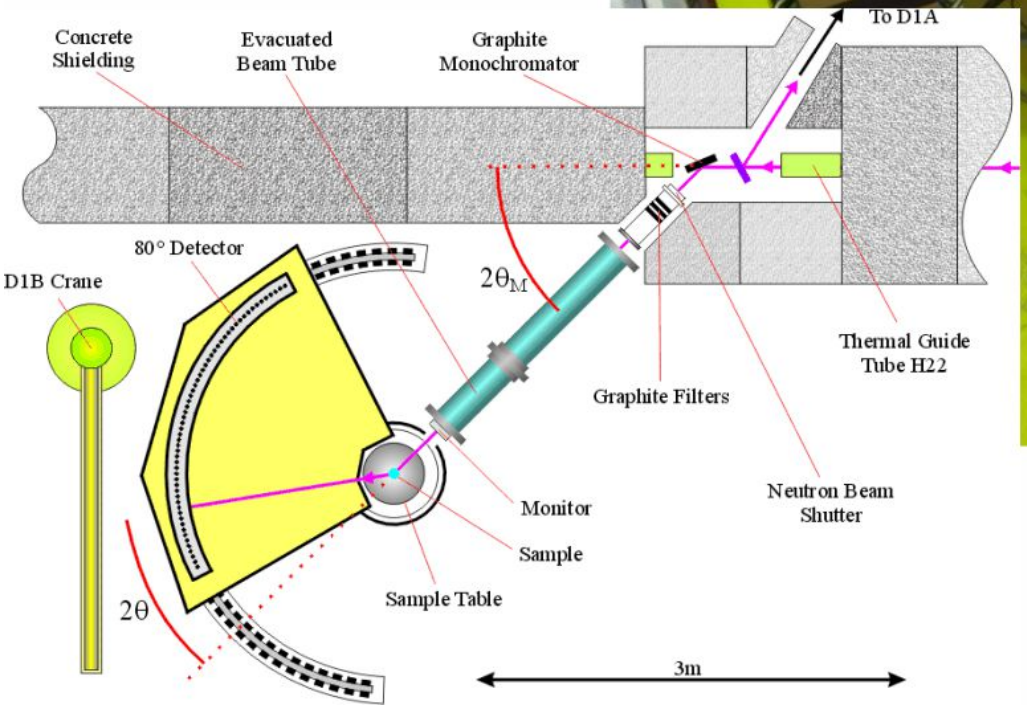


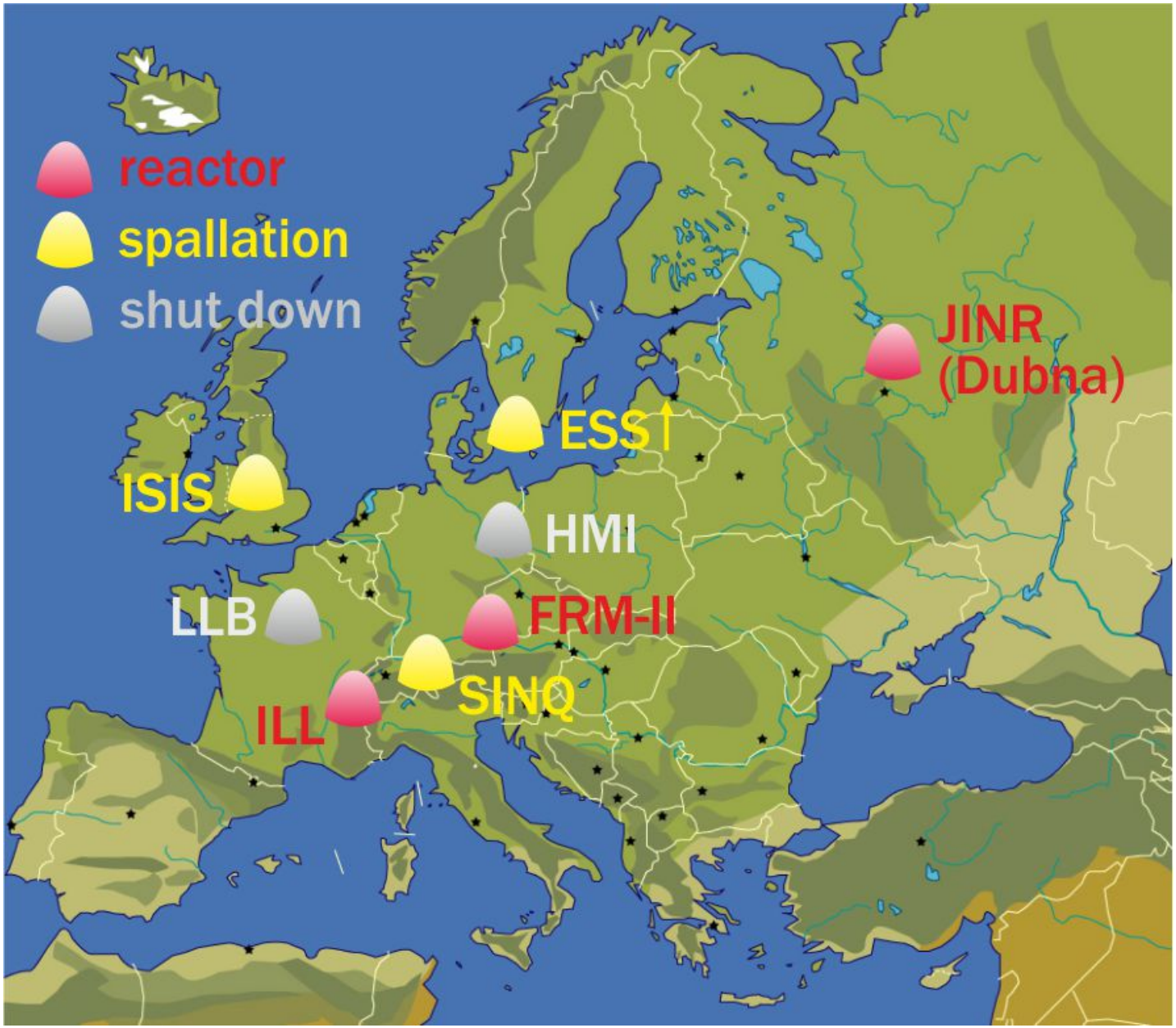
Image credits:
Kaspar Kallip (CC-BY-SA)
J. Phys. Conference Series 549, 012003 (2014)
Birkbeck College, UCL

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

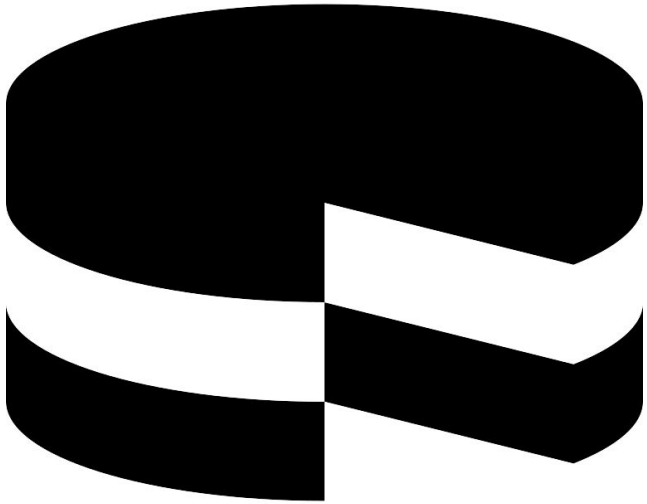
- **Spallation source:**
  neutrons may arrive in pulses
  less stable in general,
  but more environment-friendly,
  and higher flux can be achieved

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

Neutron sources in Europe



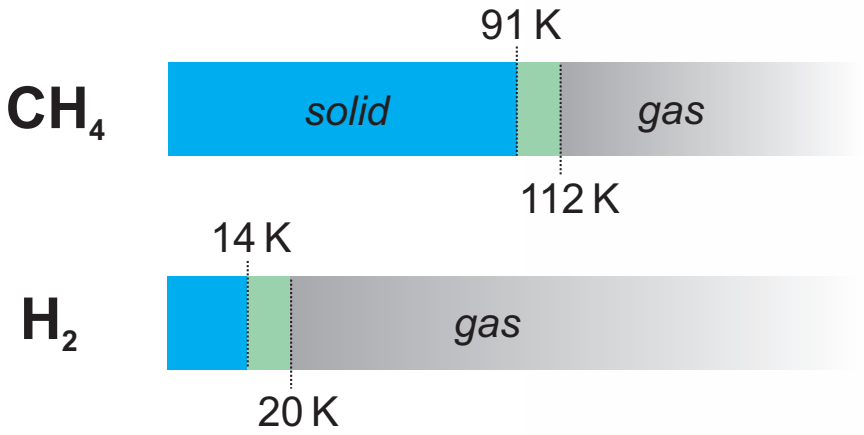
Map source: Johomaps



Material

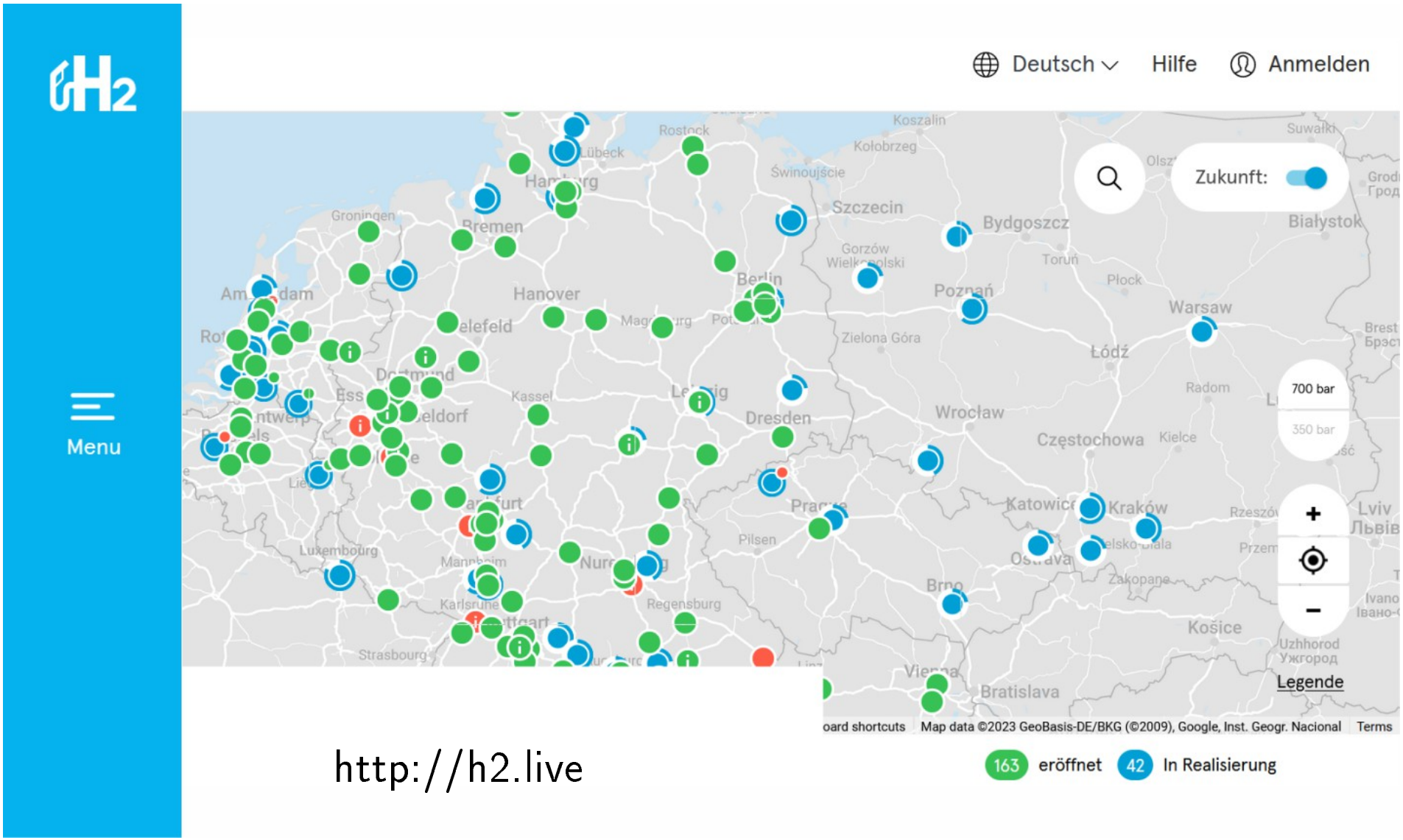
solid hydrogen

Hydrogen storage



Images: Sybille Riepe and Ogidya (CC-BY-SA)

Hydrogen tank stations



http://h2.live

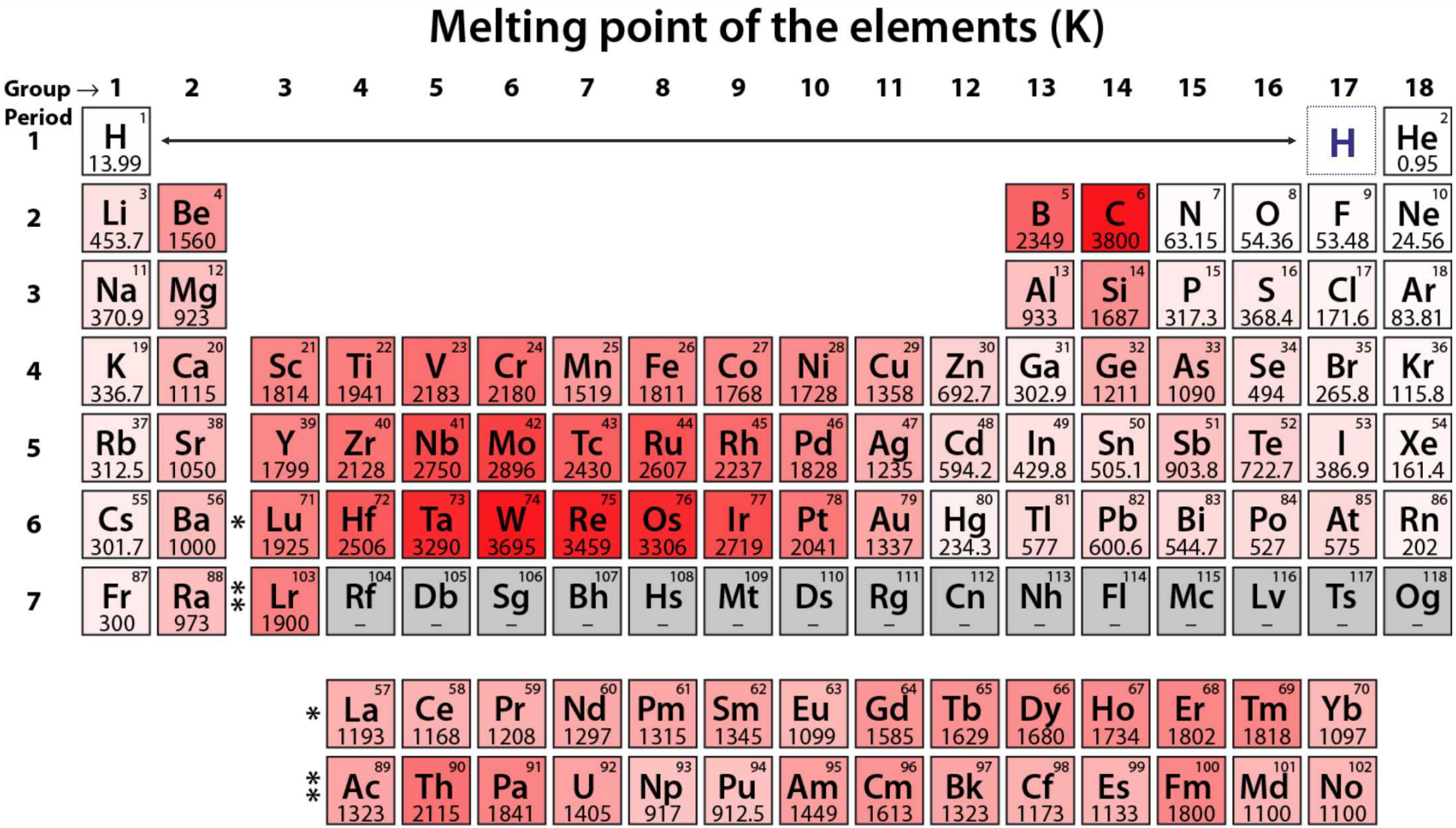
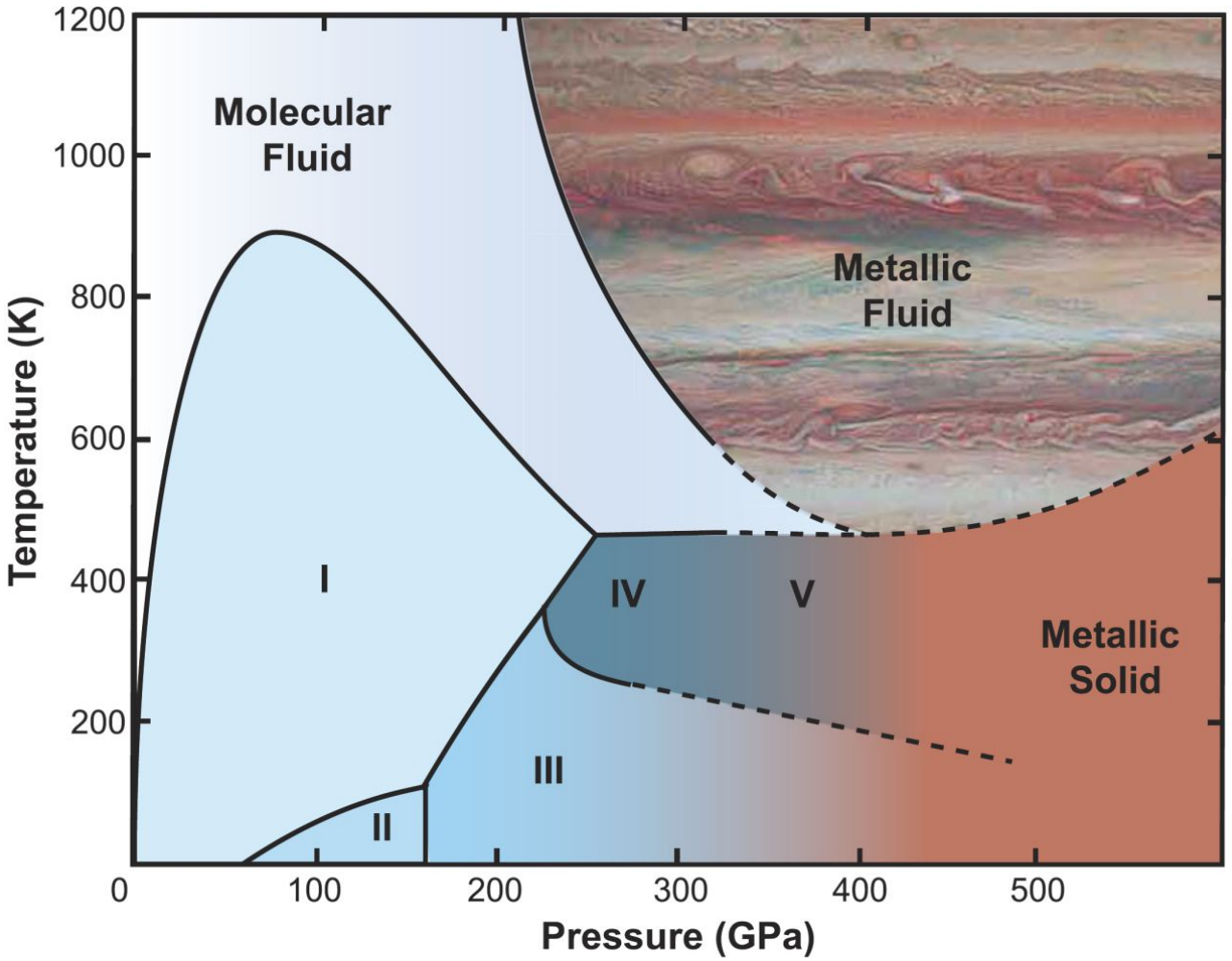
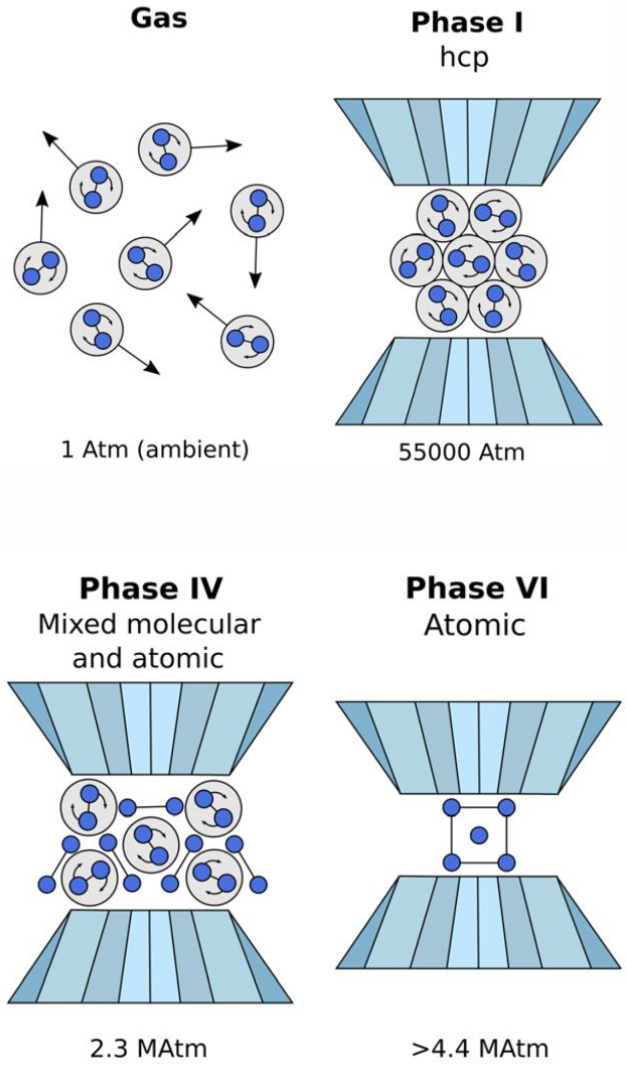


Image credit: Albris (CC-BY-SA)

Solid hydrogen





Matter and Radiation at Extremes 5, 038101 (2020)

VOLUME 21, NUMBER 26 PHYSICAL REVIEW LETTERS 23 DECEMBER 1968

METALLIC HYDROGEN: A HIGH-TEMPERATURE SUPERCONDUCTOR?

N. W. Ashcroft
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14850
(Received 3 May 1968)

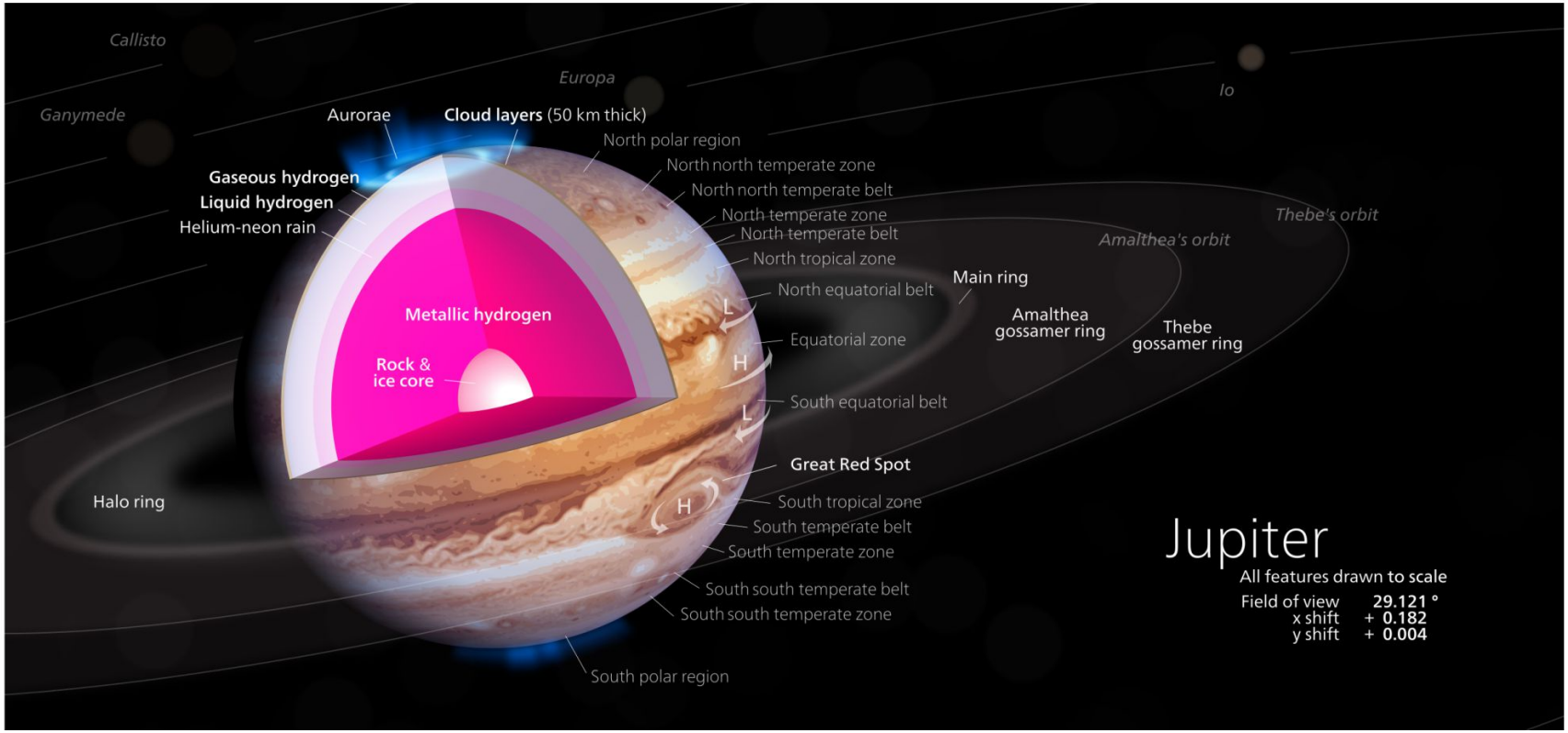
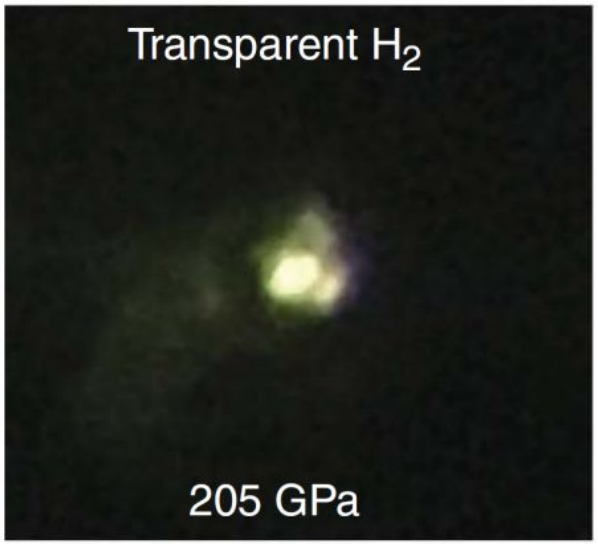
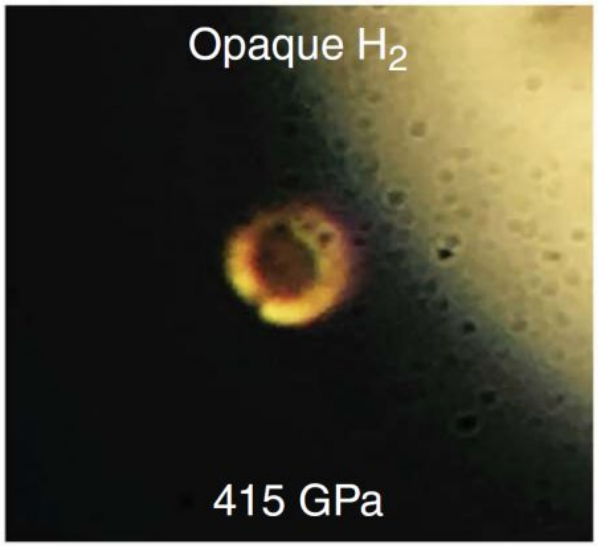
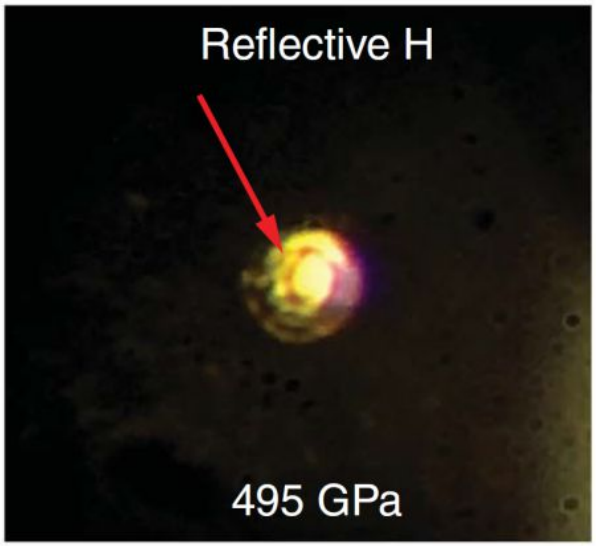


Image credit: Kelvinsong (CC-BY-SA)

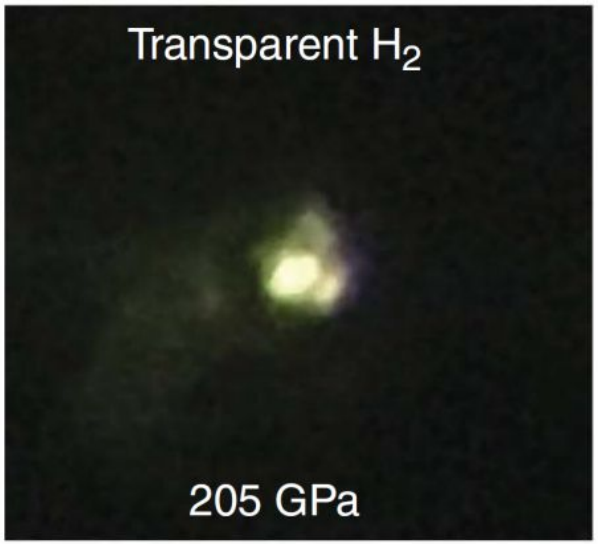


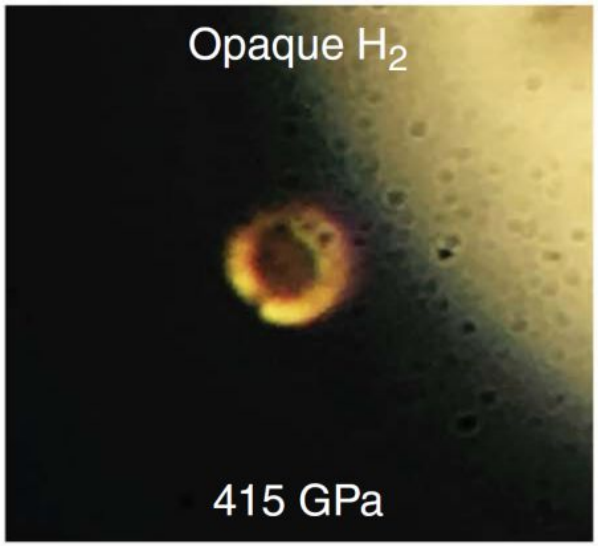


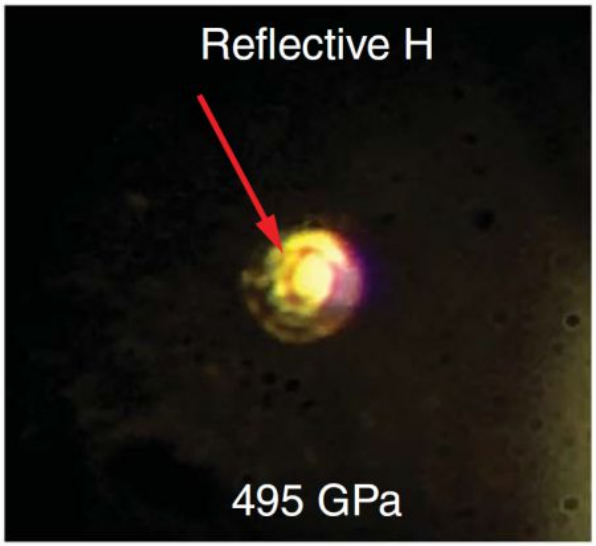


Ranga P. Dias and Isaac F. Silvera*

Science 355, 715 (2017)







Ranga P. Dias and Isaac F. Silvera*

Published: 02 February 2017

Physicists doubt bold report of metallic hydrogen

Davide Castelvecchi

Nature **542**, 17 (2017) | Cite this article

Science 355, 715 (2017)

The show must go on

"If they want to be convincing, they have to redo the measurement, really measuring the evolution of pressure," says Loubeyre. "Then they have to show that, in this pressure range, the alumina is not becoming metallic."

But Silvera says that he and Dias just wanted to get the news out before making confirmation tests, which could break their precious specimen. "We wanted to publish this breakthrough event on this sample," he says. To preserve the material, they have kept it in the cryostat; the lab has only two cryostats, and the other is in use for other experiments. "Now that the paper has been accepted," he says, "we're going to do further experiments. ■

Credits: quotation from Nature 542, 17 (2017)

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World's only piece of a metal that could revolutionise technology has disappeared, scientists reveal

Ian Johnston Science Correspondent
Wednesday 22 February 2017

INDEPENDENT

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The problem of metallic hydrogen awaits you!