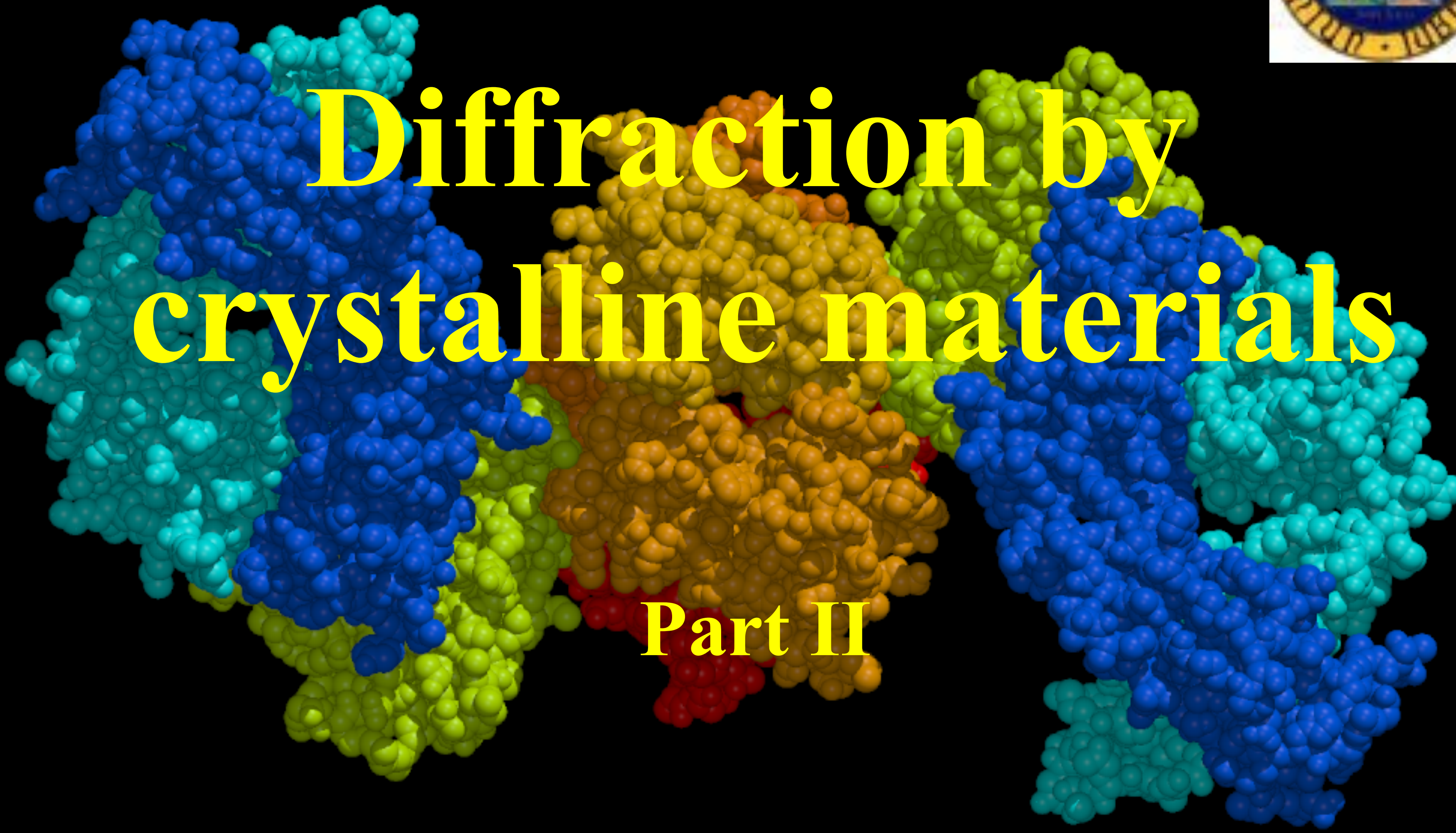
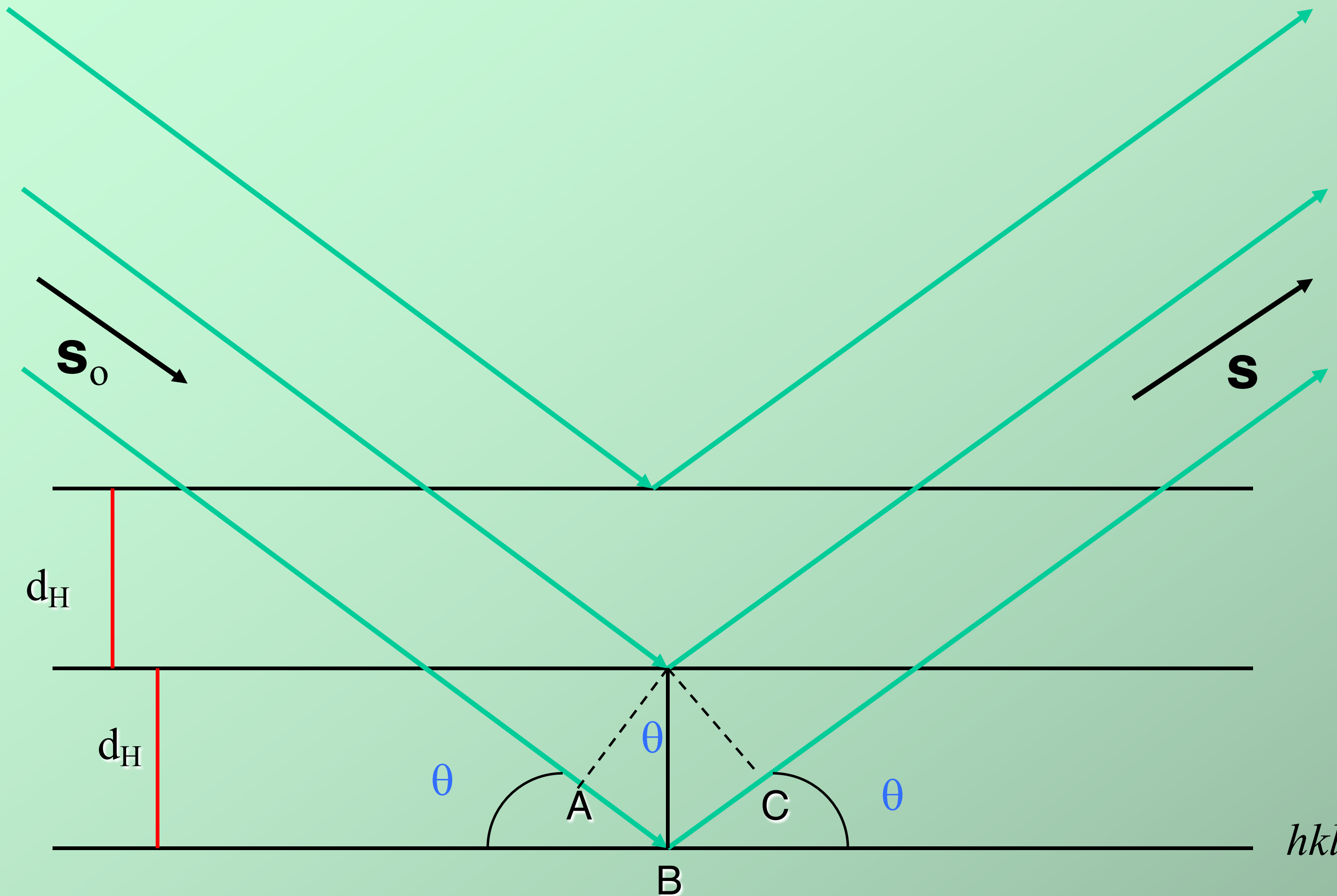
Diffraction by crystalline materials

Part II



Other useful concepts

$$2\sin\theta / \lambda = 1 / d_H = |\mathbf{s}_H|$$

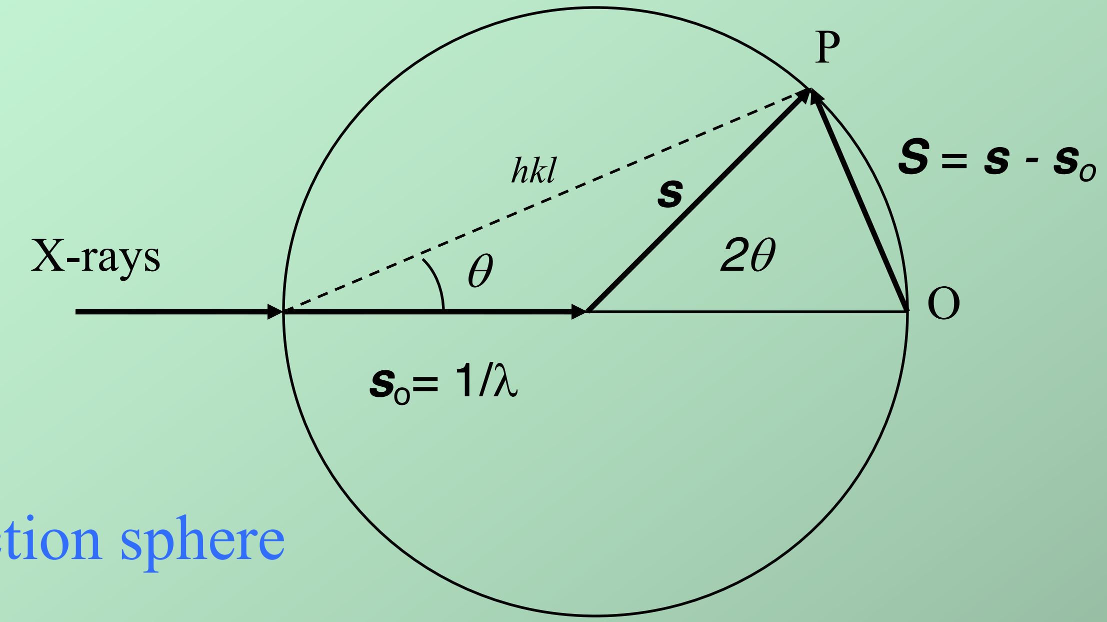


$$AB + BC = 2d_H \sin\theta = n\lambda$$

The Bragg's Law

$$2d_H \sin\theta = n\lambda$$

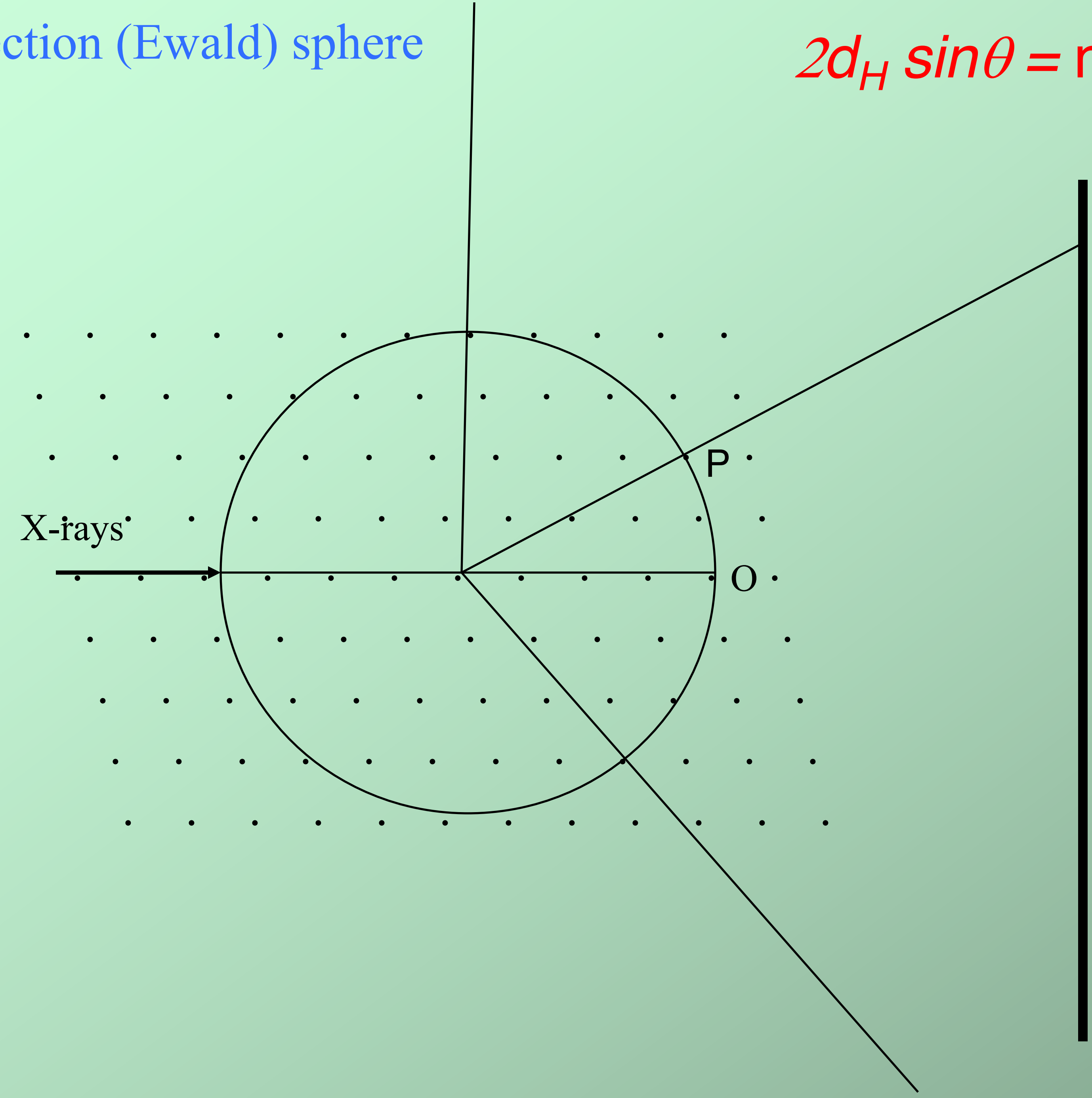
The Bragg's Law relates a distance *d* in the real space with the modulus of vector ***S*** in the reciprocal space and with indexes (*hk*l). The smallest distance *d* in the real space is related to resolution.



The reflection sphere

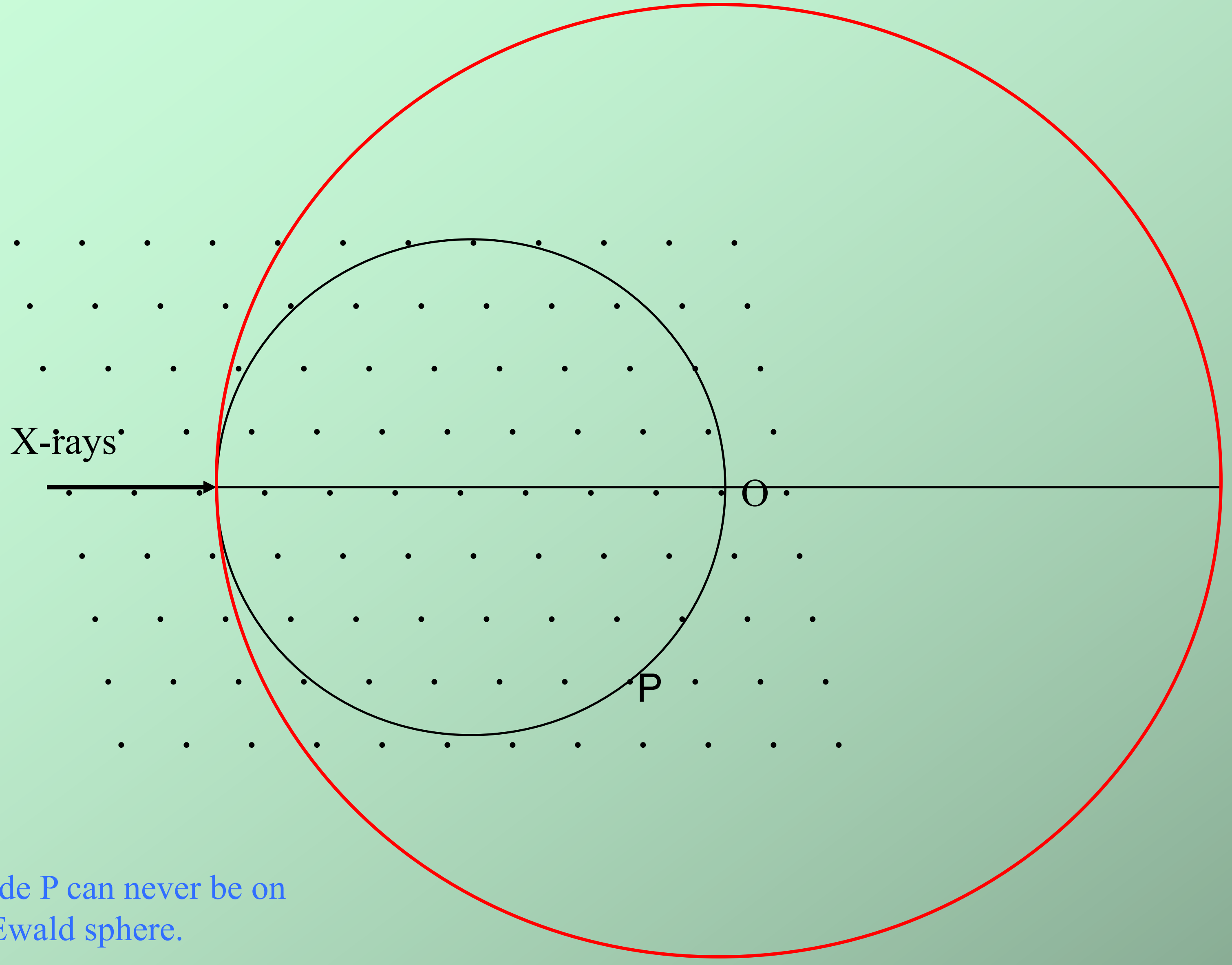
The reflection (Ewald) sphere

$$2d_H \sin\theta = n\lambda$$



The limiting sphere

radius = 2λ



If OP > 2/λ, the node P can never be on the surface of the Ewald sphere.

Resolution: the minimum *d* spacing corresponding to the maximum useful value of $\sin\theta/\lambda$

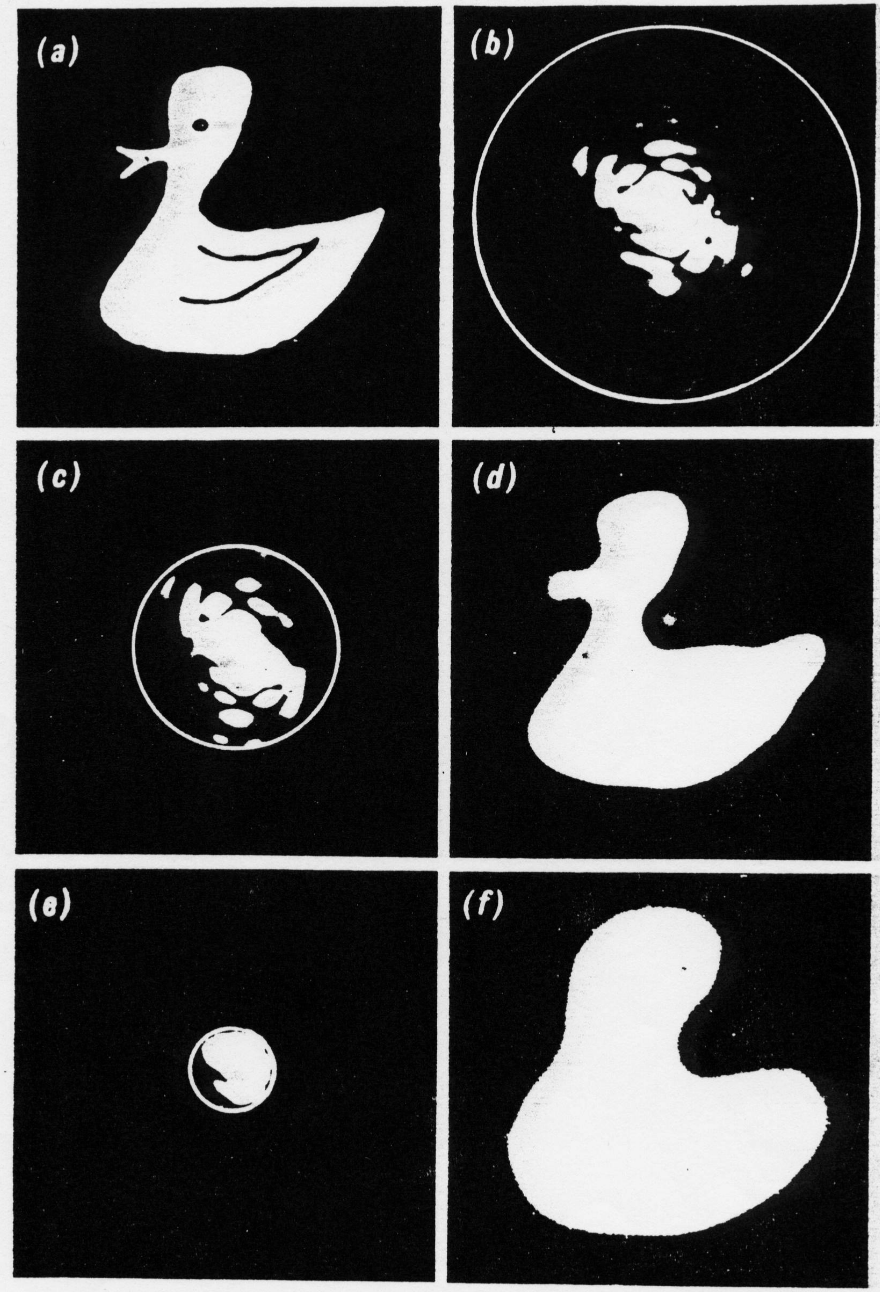
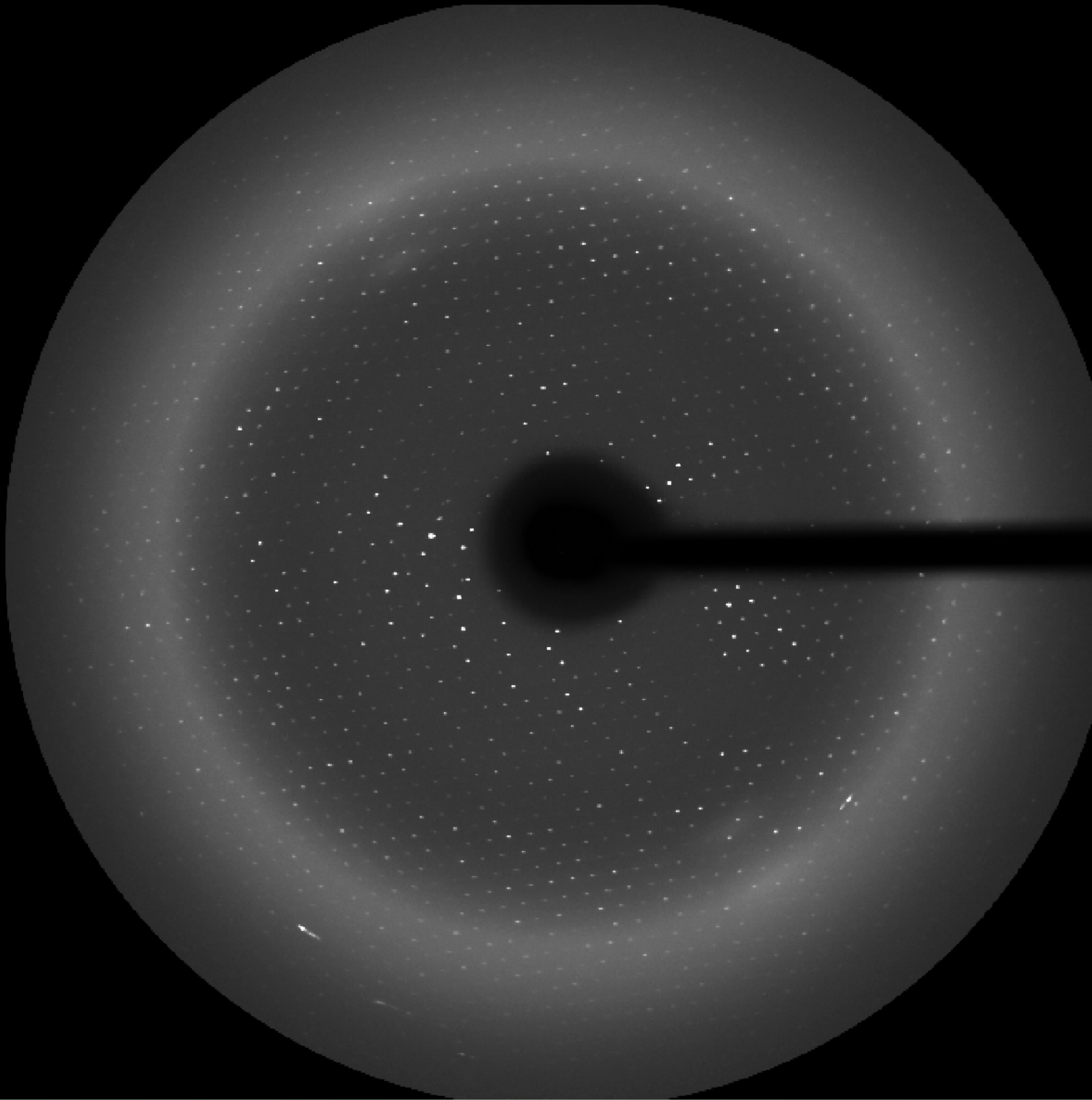


PLATE 44. (*a*) is an irregular object and (*b*) is its optical transform. (*d*) and (*f*) are the recombined images of the portions of the transform shown at (*c*) and (*e*) respectively.

See 9.7



Polarization and Lorentz factors

The coherent part of the elastic scattering of x-rays by a particle can be expressed (Thompson):

$$I_{e(Th)} = I_i\,[e^4/(m^2r^2c^4]\,(1 + \cos^2 2\theta)/2$$

Where I_i is the intensity of the incident beam. P_0 is the polarization factor when the incident beam is completely unpolarized.

$$(1 + \cos^2 2\theta)/2 = P_0$$

When the radiation source is a synchrotron, the radiation is partially polarized and the polarization factor changes accordingly.
The Lorentz factor takes into account the time a single reflection is in diffracting conditions, and its form depends from the geometry of the data collection.


Polycrystalline
samples
and others
100 µm
100 µm

Diffraction techniques can be used to measure the diffracted intensities, $I(\mathbf{S})$, on different types of samples:

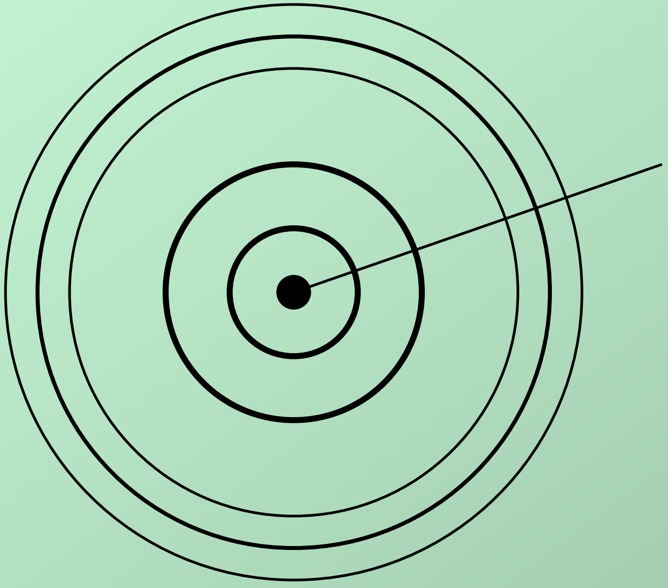
- A single crystal using a monochromatic radiation

- A single crystal with a polychromatic radiation (Laue method)

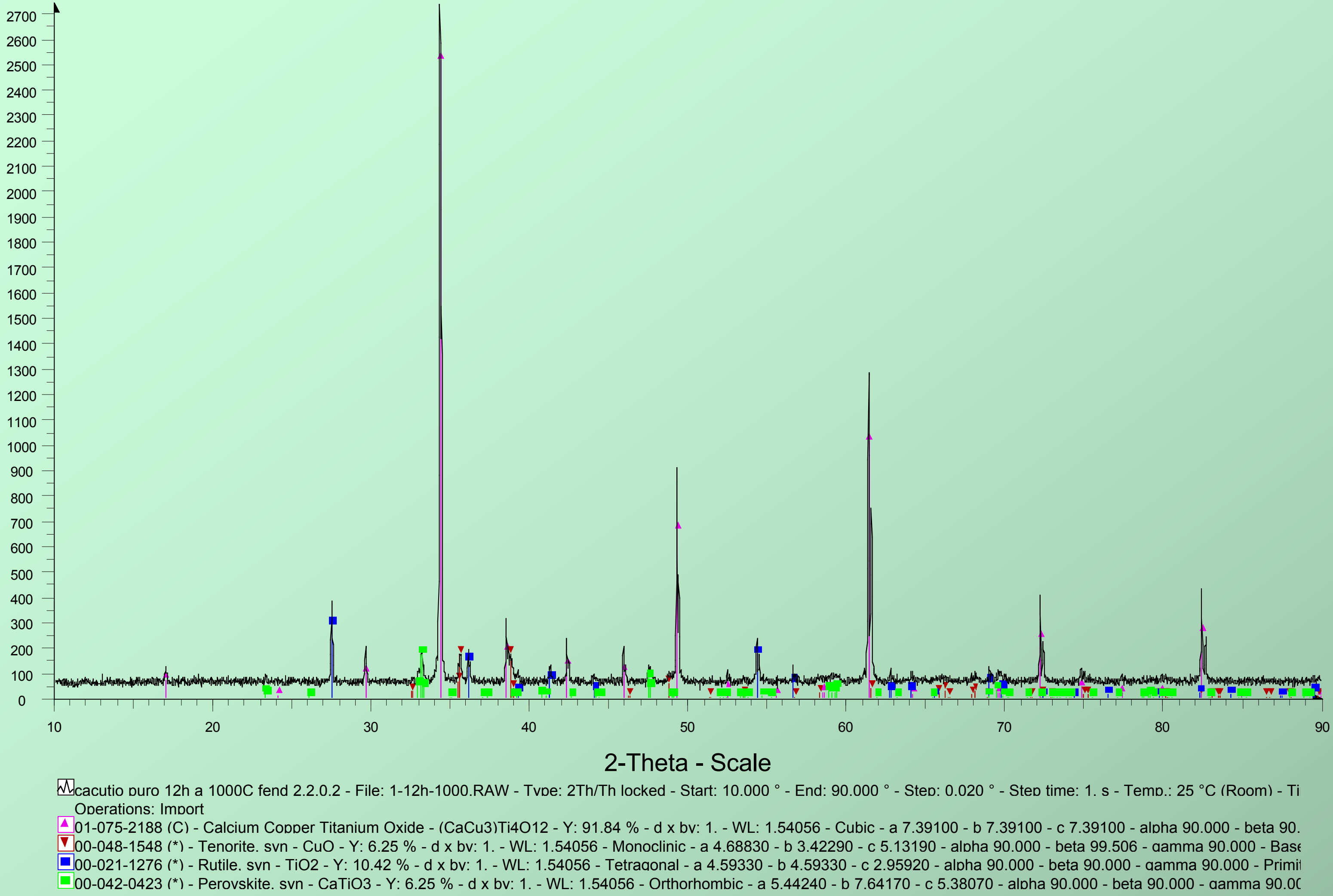
- A polycrystalline sample (powder) using a monochromatic radiation

- A sample formed by oriented polymers, i.e. with the fibers roughly oriented along one direction

A crystalline powder is formed by an infinite number of randomly oriented small crystals.
Their Fourier transform will be an infinite number of randomly oriented reciprocal lattices, all with a common origin.
Each reciprocal lattice node $\boldsymbol{S_H}$ will assume all the possible orientations, consequently they all will describe a sphere of radius | $\boldsymbol{S_H}$ |.

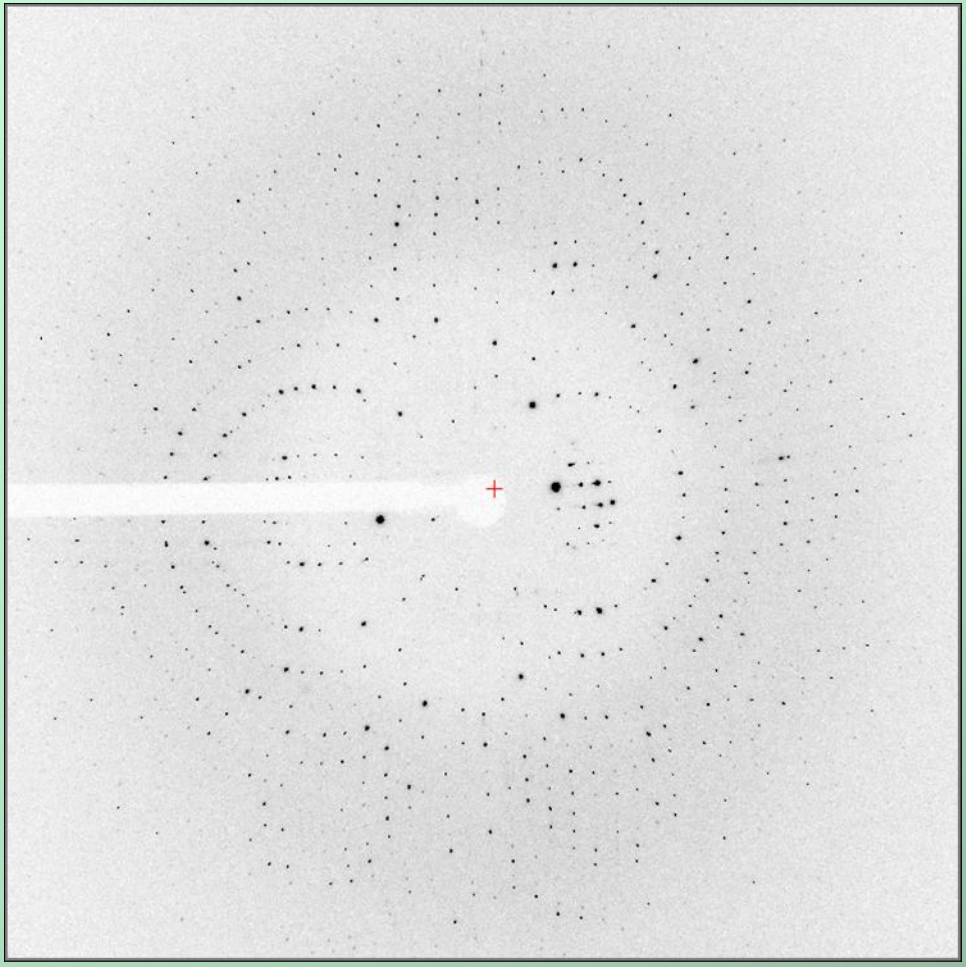


cacutio puro 12h a 1000C fend 2.2.0.2

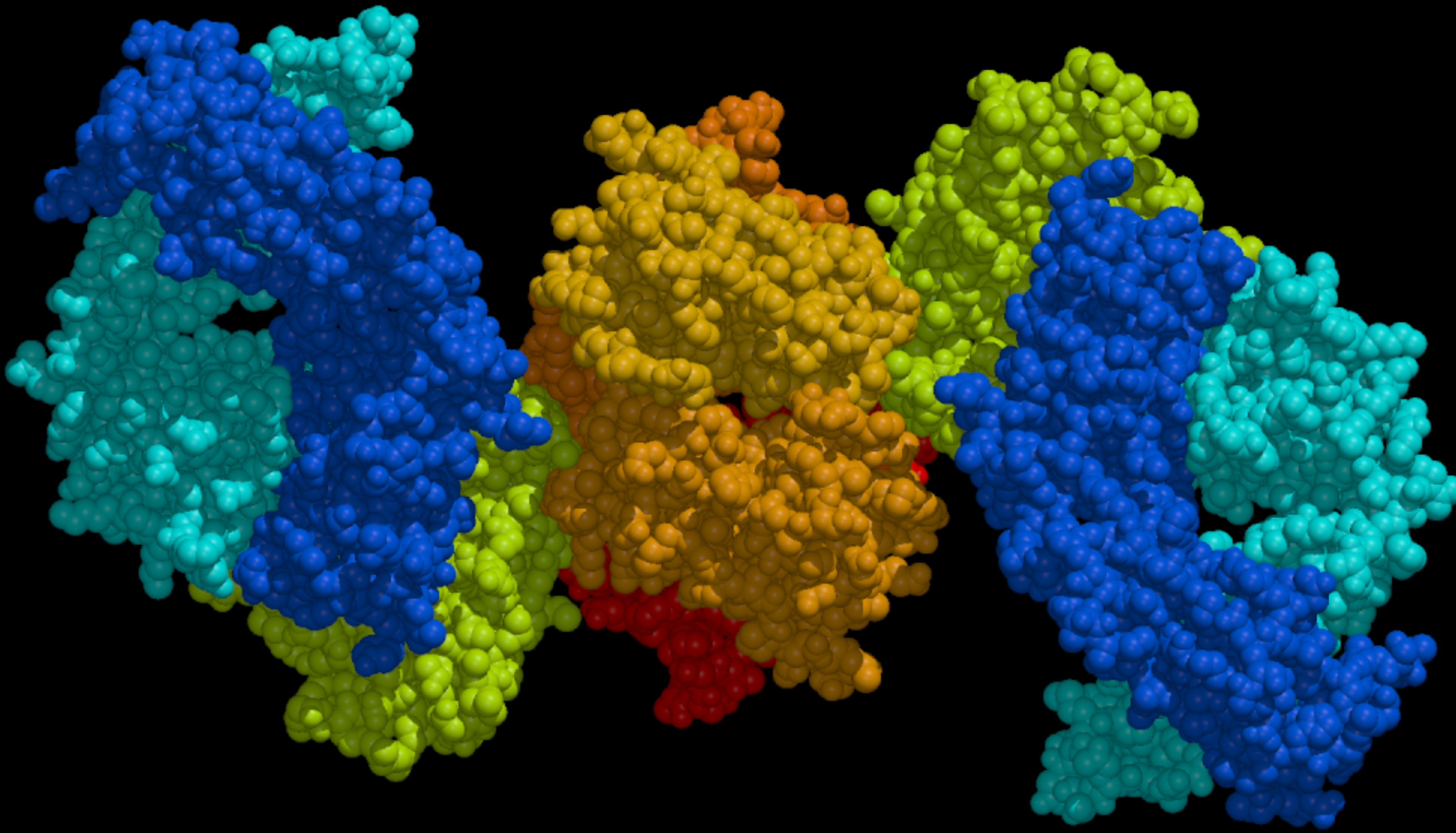


Courtesy by V. Massarotti, Pavia

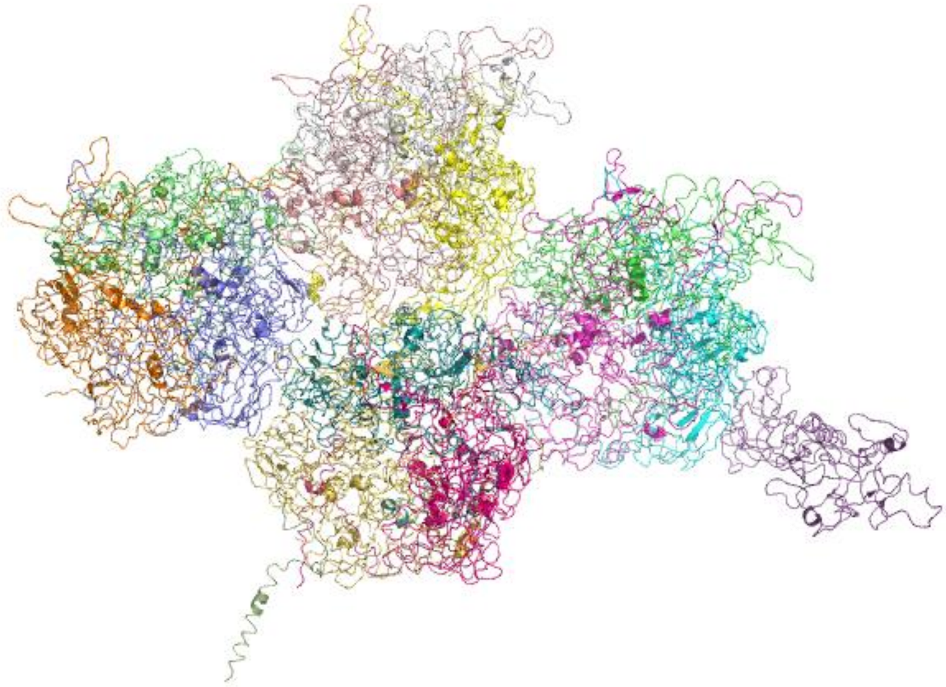
Laue diffraction pattern from hemoglobin, generated with one 160ps X-ray pulse (BioCars, The University of Chicago)

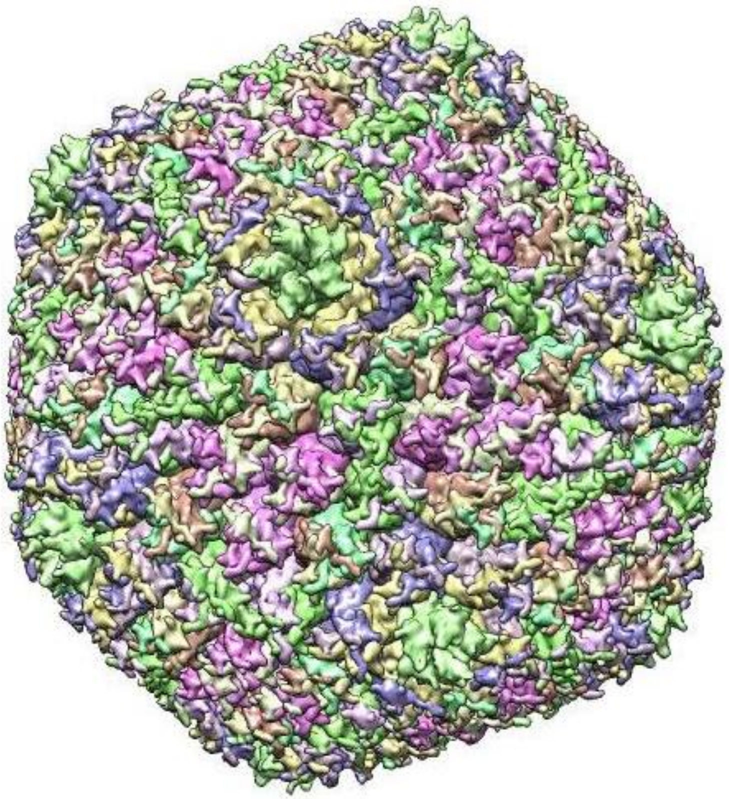



Limits
100 µm
100 µm



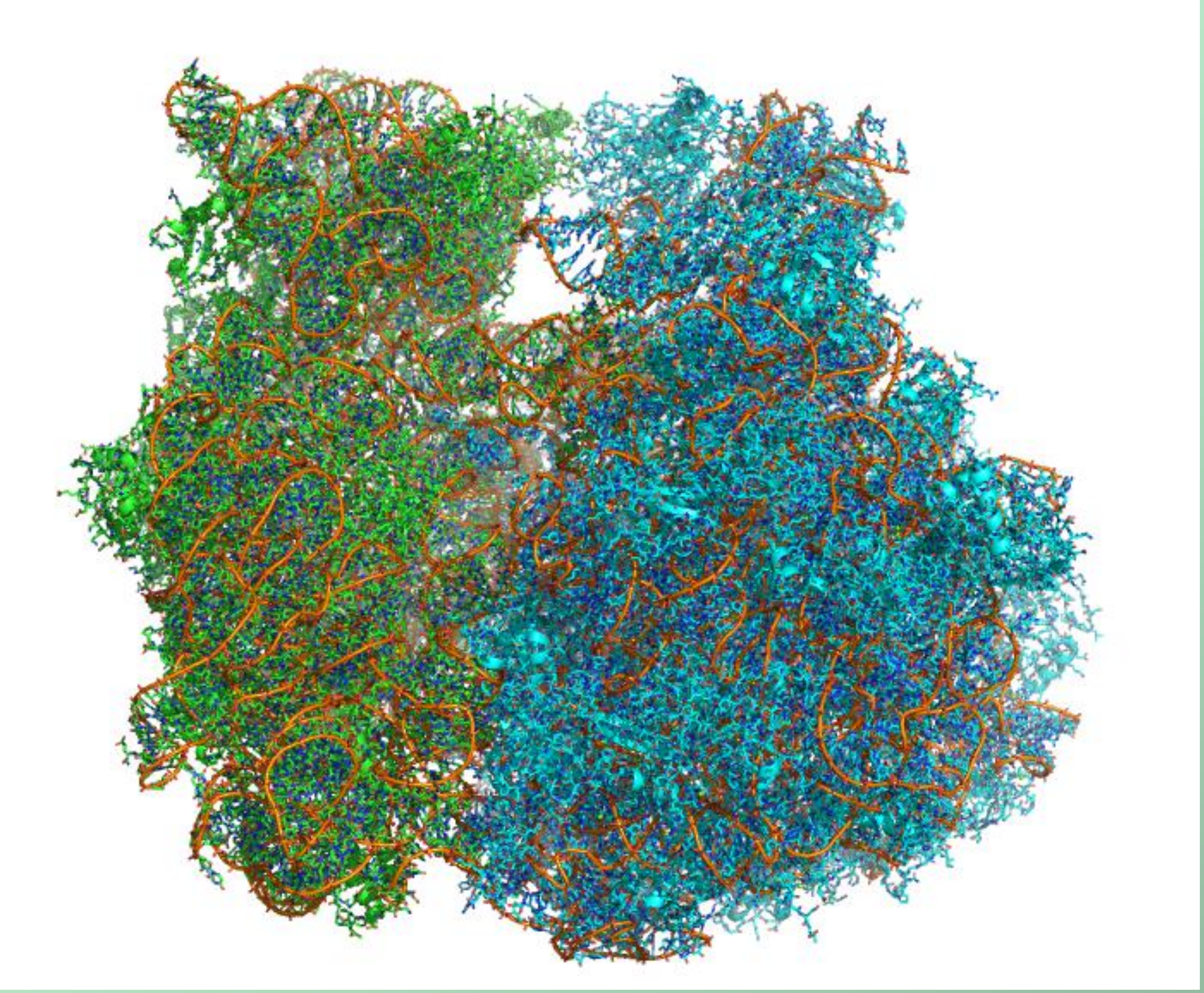
human adenovirus



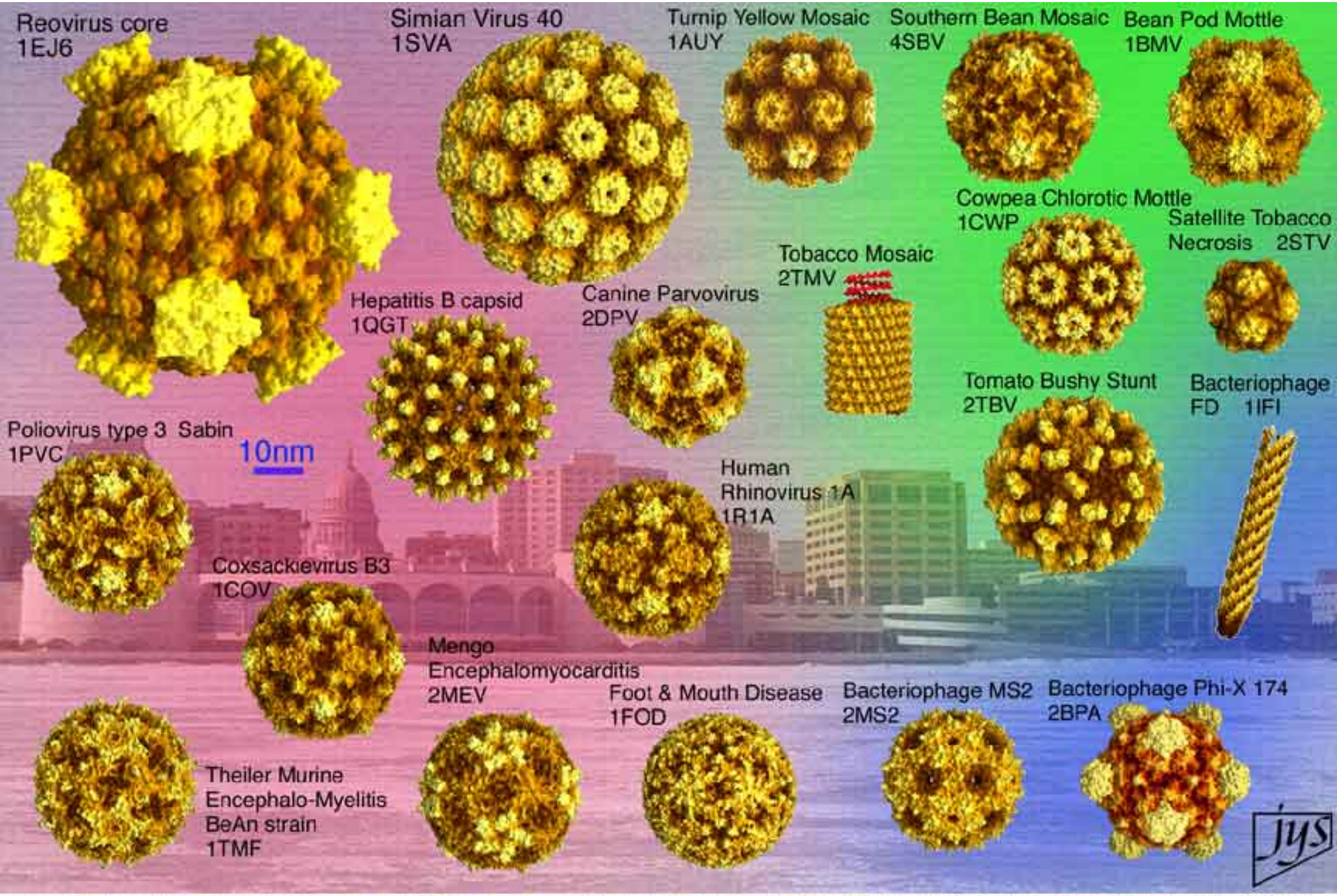


Number of atoms in a.u.: ≈ 92,000

Ribosome



Number of atoms in a.u.: ≈ 60,000



Animal (red area), plant (green area) and bacteriophages (blue area) are depicted to scale (see 10nm bar) as GRASP surfaces from published X-cray crystallography coordinates. Virus names are followed by their PDB entry code (see www.rcsb.org or mmtsb.scripps.edu/viper).
For downloadable images see also www.bocklabs.wisc.edu. Background: Madison landscape seen from Monona lake.
All Images by Dr. Jean-Yves Sgro, Institute for Molecular Virology, UW-Madison.

Cambridge Structural Database (www.ccdc.ac.uk)

1.037.850 crystal structures

Protein data bank. (www.rcsb.org)

181.969 macromolecular structures

End of part II

Which is the minimum crystal size for useful measurement of diffraction data?

$$E(hkl) \propto |F(hkl)|^2 \, V_{cryst}/V_{cell}$$

Inorganic crystal

V_{cell}=1000 Å^3
edges 10μm
10^{12} cells

Protein crystal

V_{cell} 100,000 - 1 million Å^3
edges 10μm
10^{10} - 10^9 cells