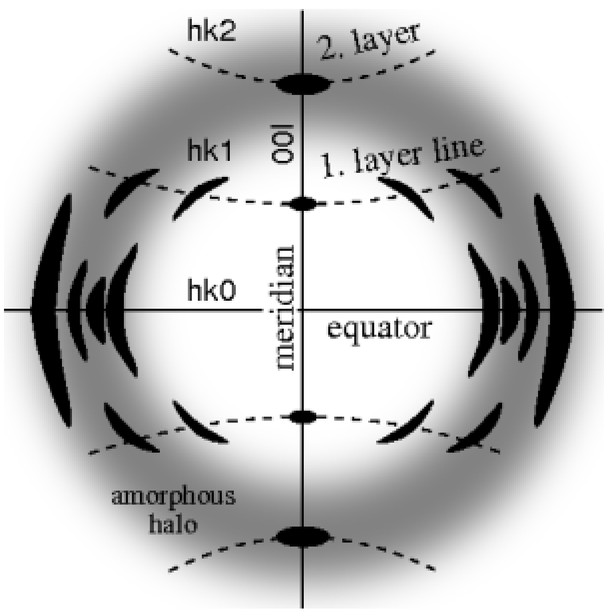
# X RAY FIBER DIFFRACTION

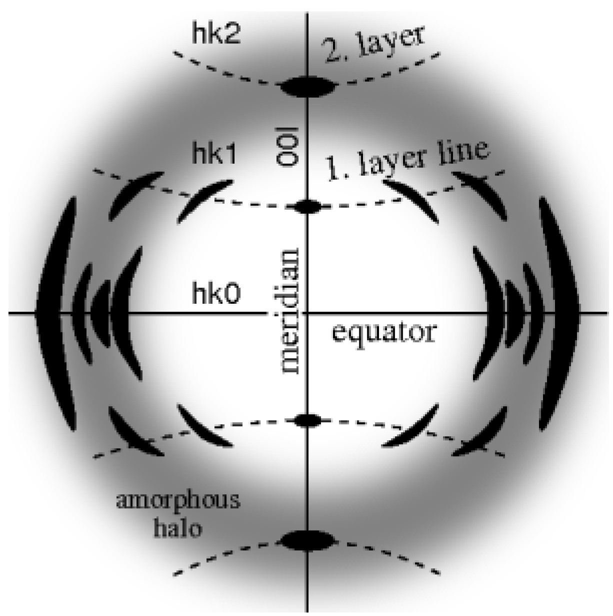
•Fiber diffraction is a method used to determine the structural information of a molecule by using scattering data from X-rays. Rosalind Franklin used this technique in discovering structural information of DNA




Ideal fiber diffraction pattern of a semi-crystalline material with amorphous halo and reflexions on layer lines. High intensity is represented by dark color. The fiber axis is vertical

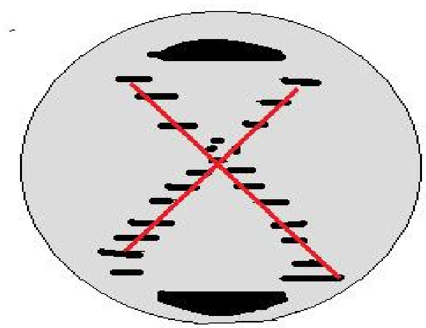
# INTRODUCTION

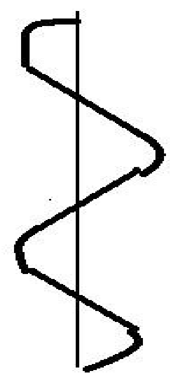
•The ideal fiber pattern exhibits **4-quadrant symmetry**. In the ideal pattern the fiber axis is called the **meridian**, the perpendicular direction is called **equator**. In case of fiber symmetry, many more reflexions than in single-crystal diffraction show up in the 2D pattern. In fiber patterns these reflexions clearly appear arranged along lines (**layer lines**) running almost parallel to the equator.



# EXPERIMENT

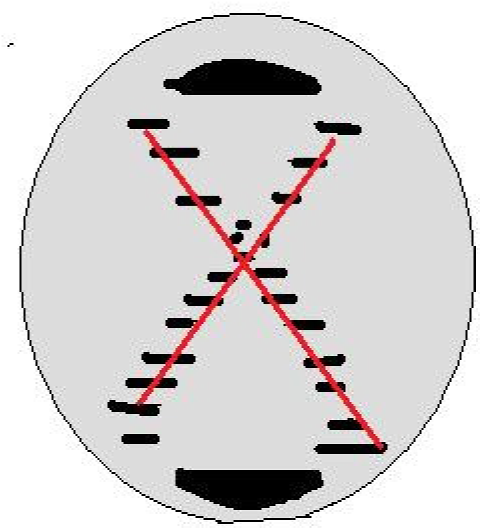
•The experiment places a fiber in the trajectory of an X-ray beam at right angle. The diffraction pattern is obtained in the films of a detector placed few centimeters away from the fiber. The fiber diffraction pattern is a two dimension patterns showing the helical symmetry of a molecule rather than a three dimension symmetry if taken by X-ray crystallography. Franklin obtained a diffraction pattern using a non-crystalline DNA fiber, and from it she deduced the B-form of DNA.

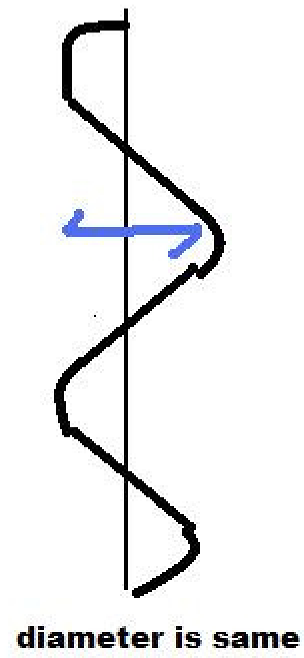




•The diffraction pattern obtained by Franklin and Wilkins showed a X pattern which hinted of a 2 stranded helical form

•They also observed that the patterns was consistent and inferred that the helix's diameter must also be consistent.





- The helical turn of DNA correlates to the horizontal lines in the picture which measures to 34 Angstroms. They also calculated that the gap between based pairs was 3.4 A as measured on the distance from the center of the X to the ends. Simple math deduced that there are 10 nucleotides per turn

- Franklin and Wilkins also showed that the sugar phosphate backbones were found to be in the outside of the helix and not inside as it was previously thought to be. They came to this conclusion because of the A and B forms of DNA. The hydrated and dry forms of DNA showed that water could easily come in and bind to DNA, a fact that could only happen if the feature showed sugar phosphate backbones being on the outside.

# SUMMARY OF FINDINGS

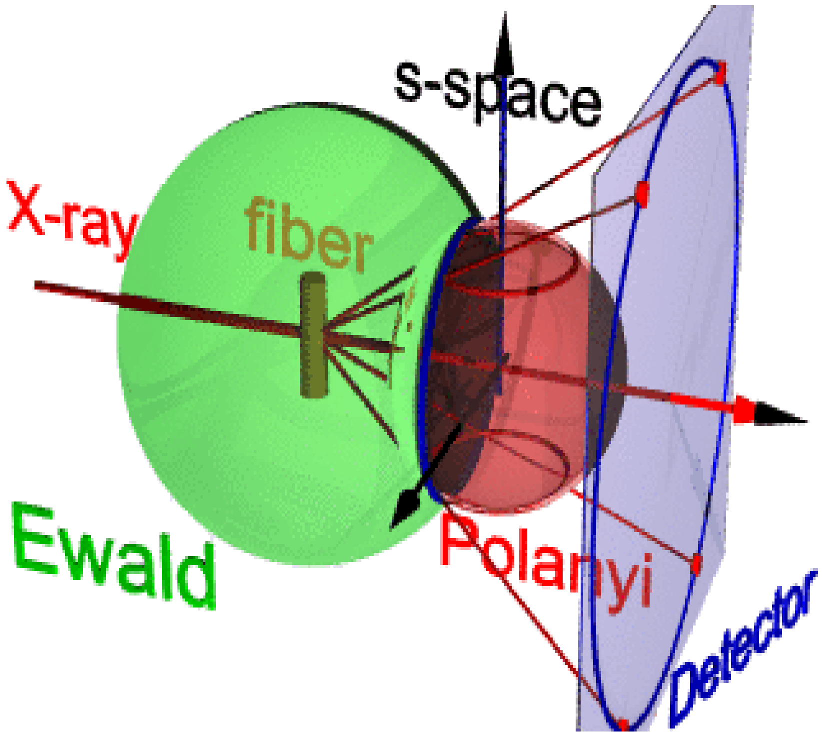
-DNA's helical structure was composed of two strands

- establish that DNA's diameter was similar throughout

- calculated that 1 turn was 34 A, distance between base pairs as 3.4A, and 10 nucleotides per helical turn

- showed that sugar phosphate backbones were located outside of the structure

# Fiber diffraction geometry

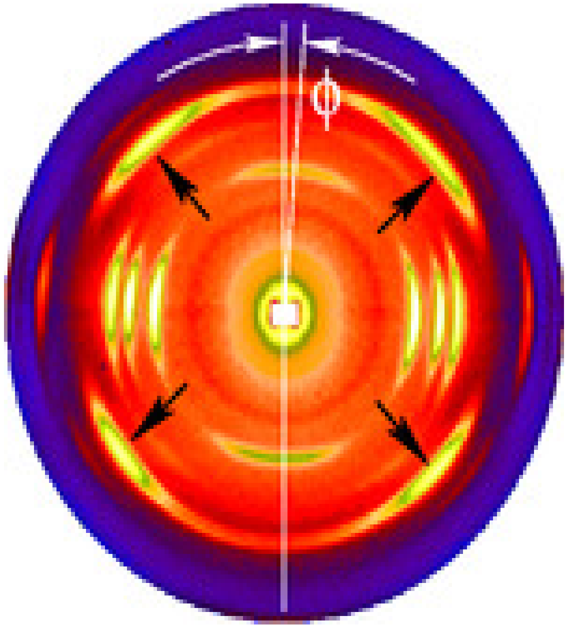



Fiber diffraction geometry changes as the fiber is tilted (tilt-angle β is between the blue rigid axis and the axis labelled *s-space*). Structure information is in reciprocal space (black axes), expanded on surfaces of Polanyi spheres

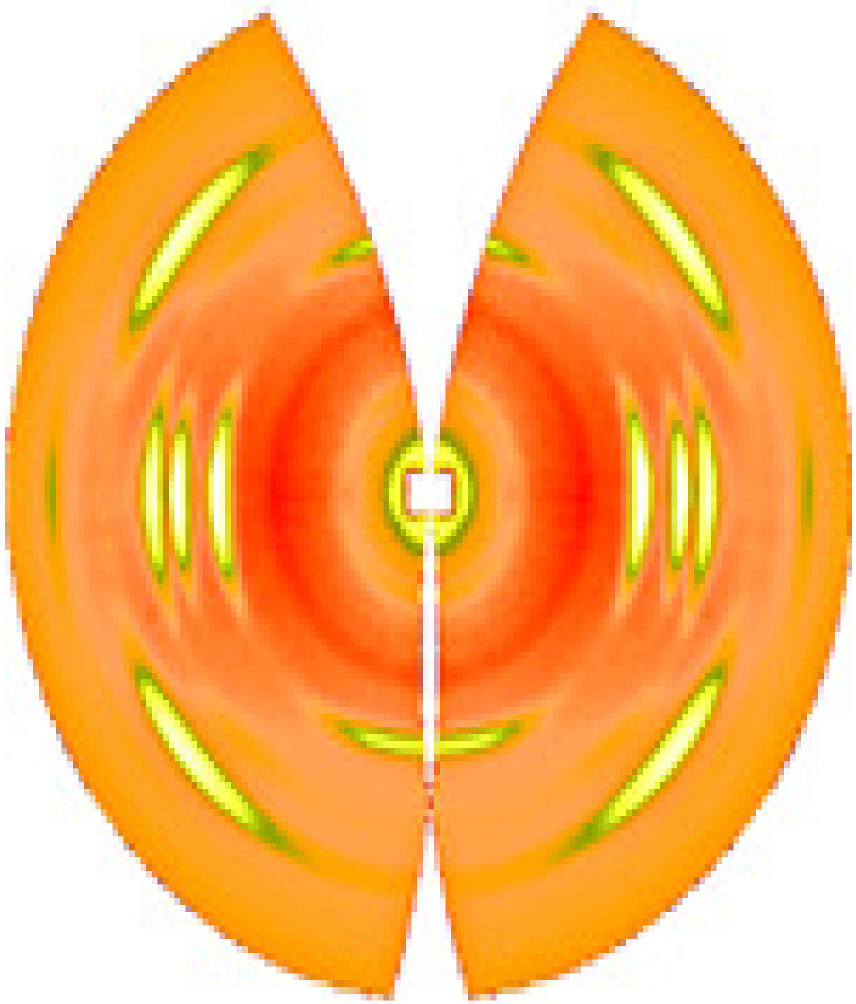
• It is based on the notions proposed by Polanyi. Reference direction is the primary beam (label: X-ray). If the fiber is tilted away from the perpendicular direction by an angle β, as well the information about its molecular structure in reciprocal space (trihedron labelled *s-space*) is tilted. In reciprocal space the so-called Ewald sphere has its center in the sample. Its radius is 1/λ, with λ the wavelength of the incident radiation. On the surface of the Ewald sphere all the points of reciprocal space are found that are seen by the detector. These points are mapped on the pixels of the detector by central projection

•In s-space each reflexion is found on its Polanyi-sphere. Intrinsically the ideal reflexion is a point in s-space, but fiber symmetry turns it into a ring smeared out by rotation about the fiber direction. *Two* rings represent each reflexion on the Polanyi sphere, because scattering is point symmetric with respect to the origin of s-space. Mapped onto the detector are only those points of the reflexion in s-space that are both on the Ewald sphere and on the Polanyi sphere. These points form the **reflexion circle** (blue ring). It does not change as the fiber is tilted. As with a slide projector the reflexion circle is projected (red moving rays) on the detector (**detector circle**, blue ring). There up to 4 images (red spots) of the monitored reflexion can show up.

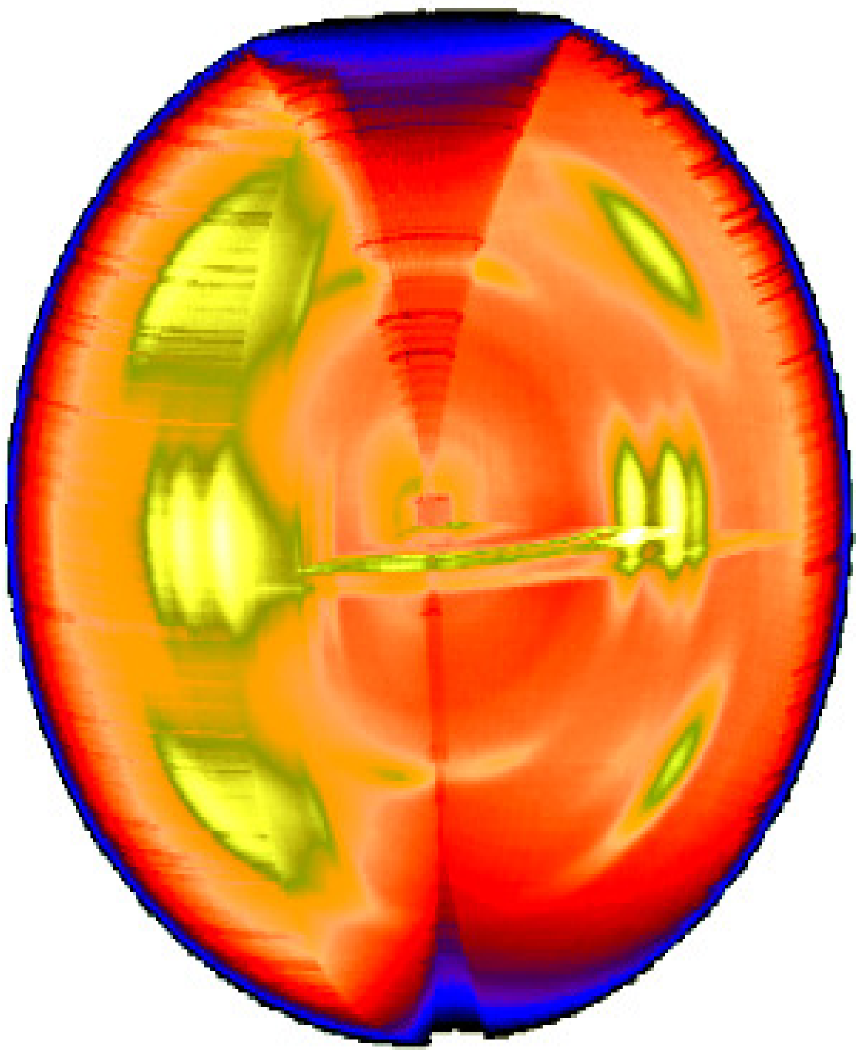
# Pattern correction




The figure shows a typical fiber pattern of polypropylene before mapping it into reciprocal space.



Fiber pattern of polypropylene mapped into (the representative plane of) reciprocal space



3D representation of the reciprocal space filled with scattering data from the polypropylene fiber


Thank You!