2. X- ray Fiber diffraction

Fiber diffraction method used to investigate the structural information of a molecule using scattering data from X-rays. This molecule is either a protein, peptide, lipoprotein, phosphoprotein, nucleic acid and bionano particles.
The theory of fiber diffraction is similar to that of crystal diffraction, however, the out-put pattern is significantly different. The crystal pattern appears on the detector is dark spots distributed over the detector. Whereas, the fiber pattern is appeared on the detector as arcs because the order in fiber is not three dimensional as it in the crystal, see Figure 9.
Within the fiber, there is a repeating unit which bounds with other units in a regular arrangement along the fiber axis. Fibers are not perfectly aligned along the fiber axis; they are overlapping over each other, which causes overlapping reflection. Therefore, the spots are spread out over the detector forming the arcs.
In a fiber diffraction, there are two main reflections responsible on the symmetry of the fiber. The first reflection is called meridional reflection (M) and the second is called equatorial (E). Meridional reflects the ordered interactions along the fiber axis, while equatorial reflects the information of the interactions perpendicular to the fiber axis.

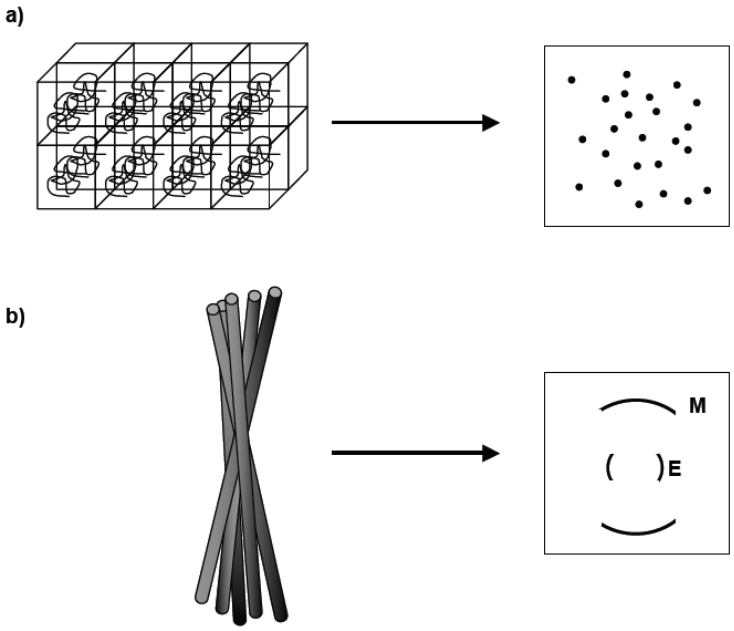

Figure 9. The X- ray diffraction scheme of a) crystal, which appears as spots and b) aligned fibers appear as arcs in meridional (M) and equatorial (E).

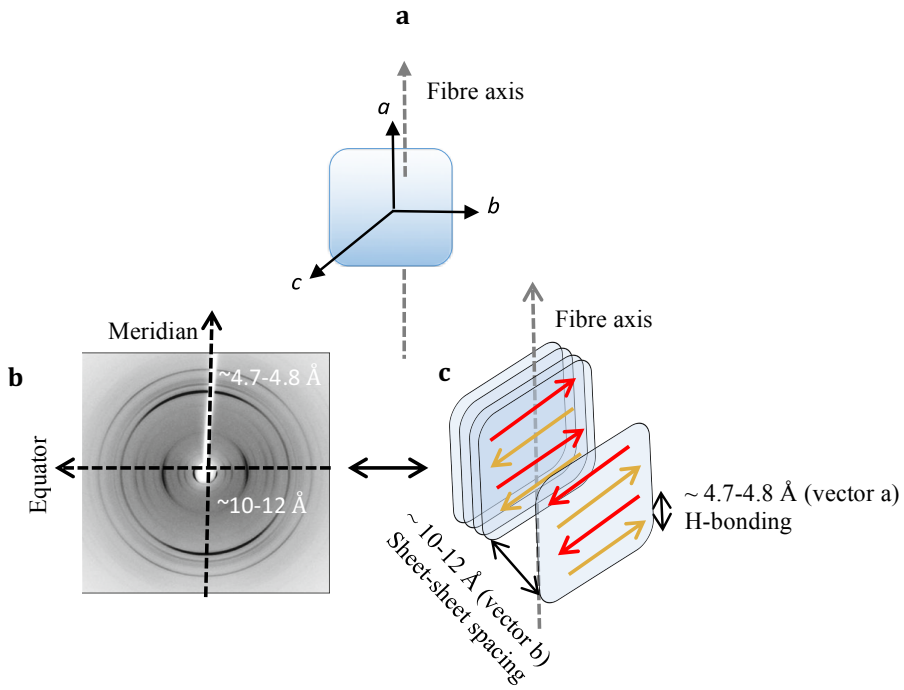

Figure 10. The diffraction pattern of cross-β structure.

The interactions along the fiber axis (direction a in Figure 10a) are corresponding to the hydrogen bonding between peptides, this distance appears on the detector as arcs in the meridional directions. Whilst, directions b and c in Figure 10a are referring to the distance between sheets and the length of the chain respectively, which appear as arcs in the equatorial direction, see Figure 8b. The molecular structure of the fiber depends on how good alignment of the fiber, which allows to collect better fiber diffraction data. Figure 10 shows a diffraction pattern of a protein called amyloid, which is related to the neurodegenerative disease such as Alzheimer and Parkinson's disease. The amyloid aggregation results from abnormally misfolding of the native protein into its linear primary structure. This one-dimensional structure will stack with another similar structure in a critical mechanism to fold into a three-dimensional quaternary structure (cross-β) called amyloid. Cross-β diffraction raises from hydrogen bonding along the fiber axis of a distance between 4.7-4.8 A° (a direction) and hydrophobic, electrostatic and salt-bridges interactions perpendicular to the fiber axis of a distance between 10-12 A° (b and c directions), see Figure 10c.