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X-ray diffraction

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One of the oldest applications of X-rays is the diffraction from crystals. Less than 20 years after the incidental discovery of X-rays, this phenomenon could be adopted for developing a technique able to reveal the inner content of crystals at atomic level. Noteworthy, at that time (ca. 1915) the quantum theory was not fully developed yet, and the X-ray diffraction experiments were expected to reveal not only the distribution of atoms in crystal structures but also the very nature of the electron density distribution.

Despite its age, X-ray diffraction remains the elective technique to reveal the structure of solids, being them molecular, polymeric, metallic or ionic.

However, as anticipated by Bragg, one can obtain much more from X-ray diffraction. Because X-rays interact with electrons, one can not only determine the position of atoms in the structure but also the accurate distribution of electrons around the nuclei or otherwise the electronic structure of transient species when the samples are subject to stimuli with a radiation.

Clearly, mapping finer details of electron distribution requires combination of powerful sources, efficient detectors, and more sophisticated models. In this respect, Synchrotron X-ray is considered the golden star source for extracting the most comprehensive information from X-ray diffraction. Compared to sealed tube used in laboratories, some important features make synchrotron particularly attractive: the high brilliance (which means even weakly scattered intensities are measurable); the large coherence (which means that aberration depends only on the sample); the tuneable energy (which enable to extend the resolution, if needed, or to optimize the contrast); the possibility to achieve a very small focus (which means that even small crystals can be measured).

For these reasons, Synchrotron X-ray diffraction has become a powerful technique able to respond to the needs of crystallographers for studies concerning molecular chemistry, biochemistry, mineralogy, and solid stat physics.

In this lecture, we present the principles and applications of X-ray diffraction in general and Synchrotron X-ray diffraction in particular.