

X-ray diffraction in crystals and powders

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In this lecture the diffraction of X-rays by crystalline solids will be briefly summarized. A very concise description of the main characters interacting in the play will be presented first: the crystal and the X-rays. The mathematical tools needed for an elegant and concise treatment of X-ray diffraction will then be introduced, in order to give a more detailed account of what is the nature of the interaction of X-rays with matter, starting from their scattering by an electron and ending with their diffraction by crystals. We will then see how X-ray diffraction can be exploited to obtain structural information at different levels. Finally a brief account of X-ray diffraction by polycrystalline samples will be presented.

A more detailed list of the arguments is the following:

1. Mathematical description of a crystal. The lattice function, the Dirac δ function.
2. Fourier transforms. The Fourier transform of a δ function. The concept of convolution.
3. X-ray diffraction. Thomson scattering. Interference of scattered waves. Scattering by matter. Diffraction by a crystal.
4. The phase problem. The Patterson method.
5. The Bragg's law. The concept of resolution. The Ewald and the limiting spheres.
6. Diffraction by polycrystalline samples.

References

1. *Fundamentals of Crystallography*, edited by C. Giacovazzo, Third Edition, Oxford University Press, Oxford, 2011
2. Davide Viterbo and Giuseppe Zanotti, *X-ray diffraction by crystalline materials*. In *Synchrotron radiation. Basics, Methods and Applications*. S. Mobilio, F. Boscherini and C. Meneghini, Ed. Springer, 2015.