



## Fundamentals of diffraction

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The lecture aims at providing mathematical and physical tools for understanding the x-ray diffraction and for its quantitative treatment. To explain the physical Diffraction phenomenon, as related to Crystallography, it is important to mathematically model the various components which characterize a crystal. In particular one needs:

- a *mathematical model of the lattice*
- a *mathematical model of the crystal*
- a *mathematical model of the radiation*
- a *mathematical model of the interaction crystal – radiation.*

It is shown that:

- a) a lattice may be mathematically represented via a set of Dirac delta functions ( the lattice function). Some properties of the delta functions will be enlightened.
- b) a crystal is the convolution between the lattice function and the content of the unit cell. Some mathematical details about the convolution will be given, with examples referred to the common life.
- c) the X-ray radiation may be represented by an electromagnetic wave. The concepts of wavelength and frequency will be recalled.
- d) the Fourier transform may model the interaction radiation –crystal. Some details on the Fourier transform theory will be given, with special reference to crystallography.

In particular, since the Fourier transform experimentally provides the information we need for studying the crystal, we will give :

- i) *the bases of the Fourier Transform;*
- ii) *the Fourier transform of the lattice;*
- iii) *the Fourier transform of the unit cell content;*
- iv) *the Fourier transform of the crystal.*

The above sequence allows s to gradually move from continuous Fourier transform to discontinuous diffraction patterns.

In particular the lecture will touch in order the following topics:

- *Thomson scattering*
- *Compton scattering*
- *The beam interference and its relation with the Fourier transform*
- *the scattering amplitude of an electron*
- *the atomic scattering factor*
- *the atomic thermal factor*
- *the scattering amplitude of a molecule*
- *the scattering amplitude of an infinite crystal*
- *the scattering amplitude of a finite crystal*
- *the concept of structure factor*
- *the Bragg law*
- *the Ewald sphere*
- *symmetry in reciprocal space*
- *how to discover the Laue group*
- *the systematically absent reflections and the space group determination*