

Alice and Joseph in crystal-land

The structure of crystals could not, at the time, be seen directly with a microscope, but had to rely on diffraction. The geometry of the locations of the different diffracted beams/spots allow the structure to be represented in a virtual space which is called "reciprocal space".

Joseph Fourier

Egyptologist, scholar and administrator. Prefect of Isere in 1802, he studied the propagation of heat and needed more powerful mathematical tools for these calculations. He liscovered a complex periodic function can be decomposed into a sum of simpler functions (sine wave like), which are now known as Fourier series. This information is encoded by its Fourier transform. Researchers use the Fourier transform to "see" inside the periodic crystals Source: Wikipedia

Using mathematics to see crystals

A precise mathematical relationship, the "**Fourier Transform**", exists between the "reciprocal space", observed by diffraction, and the real structure of the crystal in "direct space".

In order to "understand" this relationship, think of Alice (in Wonderland), who has a direct view of the world of the crystal and its atoms, and that of Joseph (Fourier), who can only see those produced by the diffraction spots!

Travelling into "reciprocal space"

The direct observation of a "reciprocal space" via diffraction enabled cristallographers to see the symmetry of a crystal, the dimensions of its building block or "unit cell" and finally to "see" the atoms themselves: **the diffraction pattern is a finger print which identifies each crystal**.

To understand more...



Diffraction patterns obtained from a coherent X-ray diffraction experiment on an artificial crystal of electronic circuit. © IUCr – journals

Diffraction may appear complicated because it provides an inverse image, but this is nothing more than a superposition of sine waves, whose calculation was discovered by **Joseph Fourier** when he was the state representative "préfet de Grenoble" under Napoleon the First.



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metal powder containing crystals of various sizes. Source : G. Artioli

Joseph's vision of an object that is partially disordered, like wood or the threads of a spider's web (the spots are diffuse and large) © IUCr - journals



