X-ray and neutron diffraction

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This lecture [1] will focus on single crystal diffraction, first for the determination of a crystallographic structure, using X-rays or neutrons, second for the determination of a magnetic structure, using neutrons.

In the first part, a general introduction on X-ray and neutron diffraction is given. While X-rays interact with the electronic cloud, neutrons interact with the nucleus, yielding some significant differences between both radiations and thus making them complementary. Once this difference pointed out, both are treated together to discuss the diffraction condition (directions of the diffracted beams) and the diffracted intensities (through the structure factor). The impact of the crystal symmetries on the diffraction pattern is then focussed on: the symmetry of the diffraction pattern is that given by the Laue class of the crystal, while the use of a centered unit cell and the presence of non symmorphic space group operations both yield a systematic absence of intensity on some particular reflections, which is referred to as extinction rules.

In the second part, magnetic neutron scattering is considered. The propagation vector formalism is first explained and illustrated through various types of magnetic structures. A propagation vector $\vec{k}$ is analogous to the wave vector of a plane wave: It reflects the periodicity of the magnetic structure and the direction in which it propagates, and thus it gives the information on where the magnetic intensity is observed. The magnetic structure factor is then introduced and its peculiarities, coming from the nature of the magnetic (dipolar) interaction, are detailed.

Last, the most widely used single crystal X-ray and neutron diffractometers are presented. A few experimental examples on oxide materials are then shown, with a focus on the determination of the magnetic structure, including a brief discussion on group theory representation. At this occasion, various useful softwares and websites are also mentioned.

[1] See slides of a similar, but much more detailed, lecture (lectures II and III) given at a school of GDR MEETICC (Banyuls, 2018); website: http://gdr-meeticc.cnrs.fr/ecole-du-gdr-meeticc-school_v3/