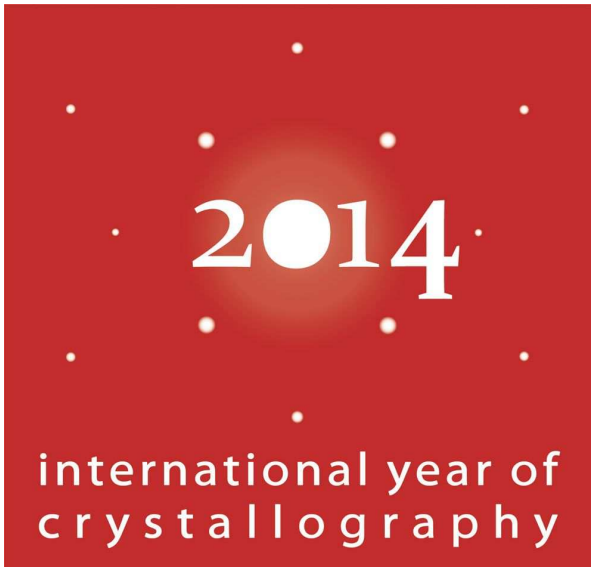
2014 – International Year of Crystallography



According to the text books, **Crystallography** is the science studying the external form, internal structure, appearance, growth and physical properties of crystals. It is located somewhere at the intersection between geology (mineralogy), physics and chemistry. The following main sections may be distinguished:

- ***crystal genesis*** studies the formation and growth of crystals;
- ***geometrical crystallography*** studies the symmetry and structure of crystals;
- ***physical crystallography*** studies the physical properties of crystals;
- ***crystal chemistry*** studies the relationship between the chemical composition of matter, its crystal structure and properties;
- ***applied crystallography*** studies methods and apparatus for growing crystals and their use in engineering.

Due to its interdisciplinarity, crystallography plays an important role in modern science as a link connecting not only chemistry, physics and geology, but also biology, mathematics and materials science.

Crystallography as a science started with the analysis of the external shape of crystals. The first notions of the symmetry of crystals were developed by *Auguste Bravais* (1848), who subdivided the types of crystal symmetry into systems. The founders of the modern mathematical theory of crystal symmetry are generally considered to be *Evgraf Fedorov* and *Arthur Schoenflies*, who, in 1891, published the theory of space groups, considering all possible combinations of symmetry elements that can be applied to a periodic arrangement of objects in three dimensions. As an experimental science, crystallography took off after the discovery of X-rays by *Wilhelm Konrad Röntgen* in 1895. It appeared that X-rays, with a wavelength of the same order of magnitude as the distances between the atoms, are deviated in a very characteristic way when they cross a crystalline substance, and that the distribution of the diffracted radiation contains all the information required to find out how the atoms are arranged. Suddenly it became possible to "see" the atoms and molecules arranged in crystal structures. The first studies of X-ray diffraction in crystals, conducted by *Max von Laue* (1912), were followed up by other famous names such as *William Henry Bragg* and *William Lawrence Bragg* (1913), and by an ever increasing number of scientists in different fields. In 2014 the crystal structures of more than 100'000 compounds have been elucidated, which has greatly contributed to our knowledge about solid state chemistry, the nature of chemical bonding, the principles governing the formation of compounds, ranging from minerals to proteins, and the relations between chemical composition, crystal structure and physical properties. The experimental methods have continuously improved; different cameras have been designed and then different models of more and more automated diffractometers. With the construction of reactors, X-ray diffraction could be supplemented by neutron diffraction. Neutrons can reveal not only the crystal structure, but also the magnetic structure of a substance. The development of synchrotron radiation made it possible to study more complex crystal structures, including those of proteins. In the very beginning the analysis of the diffracted radiation was a tedious and time-consuming work, but the computer era revolutioned also crystallography. The first universal methods to determine the atomic structure of crystalline matter from X-ray diffraction were proposed by *Arthur Patterson* (1935), and by *Jérome Karle* and *Herbert Hauptmann* (1964). Different *ab initio* methods can nowadays predict, optimize and compare crystal structures, and may be used as a complement to experimental investigations. The generally accepted idea about periodicity in crystals was harshly questioned by the discovery of forbidden symmetries, quasicrystals, modulated and incommensurate structures, in the 1970s. Also those are by now well understood and have been incorporated into modern crystallography. High-quality results, regarding not only the positions of the atoms, but also the distribution of the electron density between the atoms, can be obtained from the investigation of single crystals. But also the investigation of polycrystalline samples has progressed considerably and the universally known Rietveld refinement, developed by *Hugo Rietveld*, has become a routine tool, which allows analyzing single- or multiphase samples in powder form. The peaks in the diffraction diagrams, named after Bragg, have long

been used for phase analysis, since each substance has its characteristic diffraction pattern, but the complete diffraction diagram also contains information about the grain size, useful for example when studying nanoparticles, crystallinity, *etc.* Taking advantage of technical advances in other fields, it has become possible to analyze changes in the crystal structure under extreme conditions, for instance at high or low temperature, at high pressure, in magnetic or electrical fields, or study chemical reactions and phase transitions *in situ*.

In conclusion, few sciences have progressed so much in 100 years, and few sciences offer so many possibilities to learn more about different classes of substances. No doubt, Crystallography has well deserved to be dedicated an international year!

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