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Editorial on Crystallography

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The experimental science of determining the arrangement of atoms in crystalline solids is known as crystallography (see crystal structure). The term "crystallography" comes from the Greek words crystallon, which means "cold drop, frozen drop," and graphein, which means "to compose." The United Nations proclaimed 2014 to be the International Year of Crystallography in July 2012, acknowledging the importance of the science of crystallography. The study of crystals was focused on physical measurements of their geometry using a goniometer before the invention of X-ray diffraction crystallography. This entailed determining the symmetry of the crystal in question by calculating the angles of crystal faces relative to each other and to theoretical reference axes (crystallographic axes). A stereographic net, such as a Wulff net or Lambert net, is used to plot the location of each crystal face in 3D space. On the net, the pole to each face is plotted. The Miller index is assigned to each point. The final plot allows the crystal's symmetry to be determined.

Some crystallographically studied materials, such as proteins, do not appear naturally as crystals. Usually, such molecules are dissolved in water and allowed to crystallise slowly by vapour diffusion. In a container with a reservoir containing a hygroscopic solution, a drop of solution containing the molecule, buffer, and precipitants is sealed. The water in the drop diffuses into the reservoir, increasing the concentration and allowing a crystal to form.

After receiving a crystal, data can be obtained using a radiation beam. While several universities with crystallographic research have their own X-ray producing equipment, synchrotrons are often used as X-ray sources because they produce purer and more complete patterns.

Materials science

Materials scientists use crystallography to classify various materials. Since the natural shapes of crystals reflect the atomic structure, the effects of the crystalline arrangement of atoms are often simple to see macroscopically in single crystals. Furthermore, crystalline defects often regulate physical properties. Understanding crystal structures is an essential precondition for comprehending crystallographic defects. Materials are typically present in poly-crystalline form rather than as a single crystal (i.e., as an aggregate of small crystals with different orientations). As a consequence, the powder diffraction process, which uses the diffraction patterns of polycrystalline samples with a large number of crystals to determine structural details, is very useful.

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