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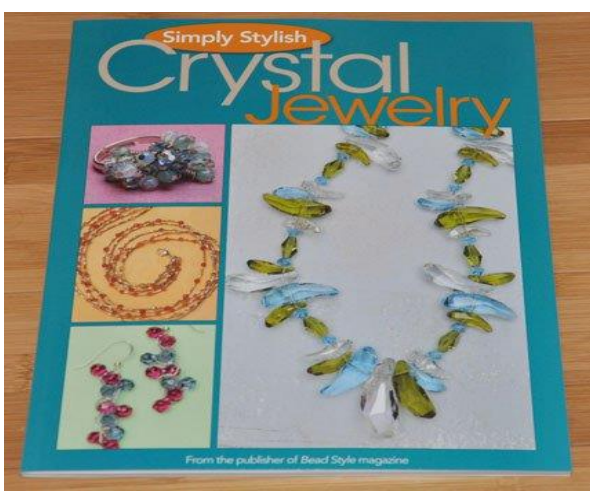
Atomic Secrets: 100 years of Crystallography

Bhawna Uttam and Manoj Kumar Singh
Department of Chemistry, Indian Institute of Technology Delhi
Hauz Khas, New Delhi, India- 110016

German scientist Max von Laue won the Nobel Prize in Physics for discovering X-ray diffraction from crystals in 1914 and led to the science of X-ray crystallography. Since then, researchers have used X-ray diffraction to work out the crystalline structures of increasingly complex molecules, from simple minerals such as quartz and diamond to high-tech materials such as graphene and complex biological structures, including viruses. With improvements in technology, the pace of discovery has been accelerated as tens of thousands of new structures are now imaged every year. One of the biggest achievement in crystallography was the discovery of the crystal structure of DNA by James Watson and Francis Crick. The resolution of crystallographic images of proteins passed a critical threshold for discriminating single atoms in the 1990s, and newer X-ray sources promise images of challenging proteins that are hard or impossible to grow into large crystals.[1]

Nature around us has an abundance of crystals. Crystals are found in a majority of rocks as minerals and also in ice, snowflakes etc. The variety of colors, symmetrical shapes, and beauty of crystals always fascinated people to know more about it. At the atomic or molecular level, crystals are ideal for studying structure of matter.[2] 28 Nobel prizes have been awarded to the projects related to the crystallography. The first structure using X-ray was determined by the father and son team of William and Lawrence Bragg in 1913 and was awarded the Nobel Prize in 1915.



X-ray crystallography has made the study of chemical bond possible which connects one atom to another. It was the greatest invention of twentieth century. Today, it is one of the foremost techniques to analyze the structures of almost anything and finding why things behave the way they do, from a metallic structure of blades of a jet turbine to the immune system fighting off viruses. Modern crystallographers are following the path invented by Braggs. The difference is that now it's being performed at larger scale with more sophisticated mathematical methods and more impressive machines. The curiosity rover is now reaching beyond our planets performing X-ray diffraction analysis of the soil on mars. There are still thousands of the complex molecules to look at and lot of more questions to answer on earth also.[3]

This year is very special as the crystallography has completed its 100 years' journey. United Nations Educational, Scientific and Cultural Organization (UNESCO) and International Union of Crystallography have declared 2014 as international year of crystallography (IYCr2014). UNESCO also celebrated 2011 as international year of chemistry and now planned to celebrate 2015 as International Year of Light. For the scientific and industrial development for developing countries there is a need to broaden the base of crystallography.[4]

Crystallography is helpful in the industries for the characterization of new products including the agro-food, aeronautic, automobile, beauty care, computer, electro-mechanical, pharmaceutical and mining industries.

The two most popular fields, in which, we have seen its application over years and years are mineralogy and drug design. Mineralogy is undoubtedly the oldest branch of crystallography since 1920. The method has been employed in determining the atomic structure of minerals and metals, and everything we know about our Earth from rocks to its geological formation, based on crystallography. Later crystallography was used to know the shape of proteins which helped in designing any drug specific to a particular protein. It has also been employed to differentiate between solid forms of a drug from one another, as the solubility alters under different conditions, thus affecting the efficacy of the drug. Crystallography is a very important tool for many pharmaceutical companies of Asia and Africa, where anti-HIV drugs are being manufactured with compulsory licensing to make them accessible to the poorest.[5] To understand active pharmaceuticals ingredients crystallography is used: Active pharmaceutical ingredients (APIs) term refers to the biologically active component of a drug product (*e.g.* tablet, capsule). There are several components in the Drug products. The APIs are the primary ingredients whereas "excipients" are other commonly known ingredients of drug products. The former are always required to be biologically safe, often making up a variable fraction of the drug product. "Formulation" is the procedure for optimizing and compositing mixture of components used in the drug. For example, if the API is a solid, then the excipients would be the liquids to formulate it, as if drug is required to have a liquid dosage form, such as cough syrup. The design criteria for any small molecule, API is usually a combination of several factors that goes beyond the intended therapeutic effect, and usually heavily encompasses both pharmacokinetic and pharmacodynamics considerations, so for this reason, API molecules have many chemical functional groups.[6]

The crystallography is very potent in tackling many challenges such as those related to health and pollution due to chemical industries. Three crystallographers Venkatraman Ramakrishnan, Thomas Steitz, and Ada Yonath have succeeded in determining the structure of ribosomes through crystallography, who won the Nobel Prize for their works. Ribosomes are responsible for the production of protein in all living cells including bacteria, so if it is impeded, cells die. This can be helpful in designing antibiotic for bacteria especially those which are resistant to the same as the target would be the ribosomes. The Crystallography also helps in reducing pollution contributed by chemical industries by making use of "green solvent" instead of chemical. The green solvent is based on ionic liquid and CO_2. It can help in reducing the mining waste and its cost of extracting the specific chemical from it.[7] Some natural crystals are given in **Figure 1**.

Figure 1. Natural crystals: (a) Dioptase (b) Vanadinite (c) Eudialyte (d) Fuchsite (e) Peacock ore (f) Wvellite (g) Spirit quartz (h) Stichtite (i) Agate

It is very interesting to see that crystallography can tackle even our basic necessities of water food and energy. It can be very helpful in water purification in poor communities, like what if we require water to be purified just once a month! Nanosponges and nanotubes could be its answer. Also crystallography can be employed in analyzing soil, structure of plant protein, which one of them are most resistant to salty environment. This will help in better productivity of food and meeting the increasing food demands. As far as the energy challenges are concerned, the crystallography can be helpful in developing new material which can reduce the cost of solar panels, wind mills, batteries, and also improving its efficiency keeping the green technology intact.

Crystallography could be indeed a revolution in each and every area of its application.

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