INTERNATIONAL YEAR OF CRYSTALLOGRAPHY

In the context of India and the North East region

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The origins of crystallography can be traced back to ancient times when man looked at gemstones, minerals and the beautifully formed salt and sugar crystals that could be obtained from substances as common as sea water and molasses. Crystals are obtained in all sizes and shapes and are found everywhere. Crystallography is the study of the macroscopic and microscopic symmetry of crystals, of their internal structure in terms of where atoms, ions and molecules are situated with respect to one another and their properties. A century ago, it was found by Max von Laue in Germany that crystals diffract, that is they bend, X-rays and this discovery was harnessed almost immediately by W. H. Bragg and W. L. Bragg, father and son, in the U.K. to internally image them. These remarkable discoveries paved the way for a scientific revolution. Today, there is literally no branch of structural science that is untouched by crystallography. The benefits to mankind have been enormous and range from the discovery of medicines and drugs, to materials that make the quality of life better for all. It is worthwhile to record here that more than 25 Nobel Prizes have been awarded in the last 100 years for discoveries in physics, chemistry, biology and medicine that depend more or less directly on this subject.

Fig.1. Diamond is probably the most glamorous crystal known to man. This is a picture of the Orlov diamond, mined in Golconda and for many years in the Ranganathaswamy temple in Srirangam, Tamilnadu, before it was taken away from India. It is now in the Kremlin in Moscow.

In July 2012, the United Nations proclaimed 2014 as the International Year of Crystallography (IYCr2014) based on a proposal by the International Union of Crystallography (IUCr), which is a 65 year old organization that acts as a forum to advance the cause of the subject. Nobel laureates like W. L. Bragg and D. C. Hodgkin have served the IUCr as presidents after they were awarded their Nobel prizes. There are more than 50 countries that are members of IUCr. India is one of the first members of IUCr and joined the organization in 1951. The IUCr has its headquarters in Chester, U. K.

IYCr2014 commemorates not only the centennial of X-ray diffraction, which allowed the detailed study of crystalline material, but also the 400th anniversary of Kepler's observation in 1611 of the symmetrical form of ice crystals, which began the wider study of the role symmetry in matter. The major objectives of the IYCr2014 are:

- To increase public awareness of the science of crystallography and how it underpins most technological development in our modern society
- To inspire young people through public exhibitions, conferences and hands-on demonstrations in schools
- To illustrate the university of science
- To intensify awareness of crystallography in Africa, Asia and Latin America
- To foster international collaboration between scientists worldwide, especially North-South contributions
- To promote education and research in crystallography and its links to other sciences
- To involve the large synchrotron and neutron radiation facilities worldwide in the celebrations of IYCr2014.

IYCr2014 is a unique opportunity for advancing all the branches of science which are closely connected to crystallography, such as chemistry, biology, physics, pharmaceutics and medicine, mineralogy, materials science, mathematics, heritage science, and all related technologies. Joint effort from IUCr, UNESCO, scientific institutions and private companies from all the above-mentioned areas are contributing to the success of the Year and for the birth of new crystallographic research centres and industrial activities, especially in the developing countries.

IUCr is organizing a number of events for IYCr2014 which will provide different opportunities for science to reach a wide audience. The variety of activities will provide opportunities to engage with: (i) the scientific community, from expert crystallographers to young researchers and students of all ages; (ii) government representatives and policy-makers, especially from developing countries; (iii) the general public. These activities are in the form of open labs and summit meetings.

Let us first consider the open labs. In many countries there is a latent crystallographic community that can be identified and strengthened. In many others, science is just too difficult to do. A fully operational crystallographic laboratory, with single crystal and/or powder diffractometers, will be situated in a hub country in the region supported by teachers and technical personnel and will conduct intensive lecture and practical courses for a week to 10 days for between 20 to 50 students drawn from several neighboring countries. Such labs have already been held in Pakistan, Ghana and Uruguay. Others are planned in countries like Ivory Coast, Cambodia and Hong Kong. An open lab is scheduled to be held in IIT Delhi later this year. Some of these labs will travel to nearby countries and are called travelling labs. This has already happened in Morocco and Algeria. The hubs will also host conferences and exhibitions, and will be actively maintained after 2014. The purpose of the open lab is manifold: in countries on the threshold of active research programs in structural science, the idea is to encourage the purchase of advanced instrumentation; in hub countries, the idea is to increase the technological base and spark interest in youngsters; in less privileged countries, the idea is to start some crystallographic activity.

IUCr in cooperation with UNESCO is also organizing a series of regional summit meetings, stressing the theme of the universality of science and also highlighting and trying to overcome the problems and difficulties in conducting first-rate scientific research in several parts of the world. These meetings would also aim to bring together countries that are divided by language, ethnicity, religion and other political factors. Depending on the interest expressed, government representatives will be invited to a round-table together with representatives from UNESCO and national and regional research centers, decision-making scientists with a leading role in their respective countries, and delegates from companies, to delineate future perspectives, possible implementations in science, technology and related industrial development, and job opportunities. These meetings form part of the IUCr's long-term commitment to nurturing crystallographic research in new parts of the globe. The first of these summits has been held in Karachi, Pakistan in April 2014 and included delegates from 22 countries, notably China, India and Pakistan. Several initiatives for regional cooperation were discussed at the summit and will be taken up for further consideration by the respective governments and the IUCr itself. There are two other summit meetings planned in Campinas, Brazil and Bloemfontein, South Africa later this year.

Fig 2. Speakers in the IYCr Summit meeting held in the University of Karachi in April 2014.

Why are these summit meetings important? While humankind has involved itself in scientific pursuits since antiquity, there is little doubt that modern science as we know it today may be traced to the Renaissance. Science leads to technology and this in turn leads to human development across the world. The connection between science, economic development and geopolitical influence is therefore quite straightforward. It is no coincidence that the development of scientifically influential ideas since the time of the Industrial Revolution, and this includes advances in crystallography, were the most prominent in the economically advanced nations: Germany, France, U.K., Russia, Japan, and finally the U.S.A.

Today, however, strategic equations in the world are changing rapidly and with the spread of education, the world is becoming "flat". Geographical constraints are not as relevant today as they were, say 50 years ago. The developing countries are catching up in all areas of science and technology. The future of science and crystallography in particular will lie in those parts of the world that have people power and economic strength. Realizing that it must make a strong commitment to parts of the world that are beginning to see an economic upswing if it is to remain viable and relevant as a scientific union, the IUCr has developed its plans for the International Year with special focus on Africa, Latin America and parts of East and South Asia that are rapidly coming into the mainstream. It cannot afford to do otherwise because these are the regions where maximum growth and future influence is anticipated. The summits are being held in these areas precisely for these reasons.

Let me now come to the teaching of crystallography and this too is an integral part of activities connected with IYCr2014. I will illustrate the problems and possible solutions as they pertain to the fascinating subject of *crystal engineering* which stands at the crossroads of chemistry and crystallography and in which active research has been ongoing for the past 25 years. However, teaching in this subject is rendered problematic because of the lack of textbooks and also because crystal engineering is an interdisciplinary subject. The division of chemistry into organic, inorganic and physical branches is traditional in teaching programs. For the undergraduate student who wishes to embark on a research career in these core areas, there is a natural continuity between what is learnt in the classroom, and what is done in the research laboratory. However, for those who enter research in areas that do not fall neatly into one of the above streams there is often little connection between one's experience as an undergraduate student and then subsequently as a research scholar. It is believed that the student will somehow acquire the basic skills needed to do research in a subject like crystal engineering from what he or she has learned in courses in organic, inorganic and physical chemistry. This is not always possible and certainly not easy.

Crystallography as a subject is insufficiently handled in course curricula, considering its pervasive influence in chemistry. With the proliferation of automated table top diffractometers and black box software, the determination of crystal structures of organic and inorganic substances seems to have become routine and automated. Challenges in small molecule crystallography today have more to do with understanding the reasons why a compound adopts a particular crystal structure and not another. Crystal engineering is part of such an endeavor because it attempts to establish packing trends in whole families of compounds. The use and relevance of crystallography in crystal engineering is much more extended than its application in traditional organic and inorganic chemistry where it is used generally only to confirm and establish chemical structure. These wider implications of crystallography as something that goes beyond crystal structure determination do not generally find a place in undergraduate teaching programs.

Let me now come to issues within India and especially as pertaining to the North East. Students, even at the secondary school level, need to be made aware of subjects like crystallography and the importance of such subjects in modern science especially the ways in which they improve the quality of life for millions of people. IYCr2014 consists also of outreach programs in schools where students are given elementary level brochures and asked to attempt simple tests that illustrate basic concepts. Already such programs have been initiated in Andhra Pradesh, Karnataka, Kerala and Delhi.

Teaching and research in crystallography is making a beginning in the eastern and north eastern regions of India. Research programs are initiated in institutions like NEHU, Sikkim University, Assam University, Gauhati University and Tezpur University, while the traditions are already developed in IIT Guwahati. It is to be hoped that there will be a networking of these universities so that greater regional cooperation will ensure mutual benefit. We are a growing country and need to help one another. It is not possible to acquire all possible scientific facilities in all possible places. There needs to be a much greater degree of inter-dependence among teaching and research institutions. This is especially the case in the north eastern part of India which is far flung and also geographically separated from other parts of the country. A case can also be made for greater academic interactions between universities in the North East and institutions in neighboring countries like China, Myanmar, Thailand, Vietnam, Cambodia and Malaysia. The north eastern part of our country certainly had many beneficial interactions with this region but unfortunately much of this came to an end after 1947. Science is a truly international activity and it works best when scientists can cross borders in an unhindered manner. It is also one of the aims of the IYCr2014 to bring nations together with science. The language of science is universal and transcends political barriers. With the current political changes in India, it is certainly hoped that we would be able to assume our legitimate leadership role in science in South East Asia.

(1) The World is Flat. A Brief History of the 21st Century, T. L. Friedman; Farrar, Straus and Giroux, New York, 2005.
(2) Crystal Engineering. A Textbook, G. R. Desiraju, J. J. Vittal, A. Ramanan; World Scientific, Singapore, 2011.

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