FUN WITH CRYSTALS, LIGHT AND SYMMETRY – IYCR OUTREACH ACTIVITIES

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The importance of crystallography was recognized by Nobel Prizes to Max von Laue in 1914, and Sir William Henry and William Lawrence Bragg in 1915. At the centennial of these events, insights gained from crystallographic experiments have revolutionized virtually all science and engineering disciplines, and benefited society through advanced materials, drugs, an amazing understanding of the human body and many more aspects. Yet few non-experts have much of an idea of what crystallography is, or why its study and use will remain important in the future. During this International Year of Crystallography 2014, the ACA is reaching out to bring crystallography to everybody in an attempt to improve recognition and appreciation for our science, and to attract the next generation of crystallographers to this field.

1. THE INTERNATIONAL YEAR OF CRYSTALLOGRAPHY

The idea to declare an International Year of Crystallography was developed several years before we actually got to celebrate IYCr2014. Based on historic events, the years 2012 through 2015 are all centennials of important crystallographic discoveries or awards, making the entire 4-year span a great time to reflect on the origins of our field. While crystallography is a much older science, which was developed by mineralogists like Steno, Haüy, Miller, Bravais, Hessel, Feodorov, Schönflies, Barlow and many others, the birth of modern crystallography as we know it can be dated to 1912, when Max von Laue, Paul Knipping and Walter Friedrich obtained the first diffraction pattern of copper sulfate pentahydrate. Soon after, in 1913, Sir William Henry and his son William Lawrence Bragg published their famous “Bragg’s law”, and reported the first crystal structures solved by X-ray diffraction. These milestones were rapidly recognized through Nobel Prizes in Physics to von Laue in 1914 and the Braggs in 1915.

International years are obviously an opportunity for those associated with the respective topics to celebrate. But they are even more so an opportunity to get others to learn about specific fields, gain an appreciation of why they are important, and to hopefully capture the attention of those who will one day choose these topics as the focus of their own studies.

Crystallography is a field that has affected virtually every science and engineering discipline, and through this contributed to a large number of beneficial discoveries for society. Yet, very few non-specialists could define what it is, and the most common answers relate to gemstones. The fact that crystallography forms the basis for knowing the atomic level structure of solids is unknown or forgotten by many, even by other scientists and engineers who use such knowledge of atomic level structure and the resulting properties of materials in their own research. Thus this International Year of Crystallography is our chance to proudly claim the accomplishments of our science, and to introduce all age and education levels to fun and exciting crystallographic topics.

In the long run, we hope to leave a legacy that will result in lasting recognition and appreciation of our field. This will be crucial to ensure both continued funding for crystallography related research, and for attracting and training the next generation(s) of crystallographers into the field.

2. FUN WITH CRYSTALS – THE OBVIOUS SIDE OF CRYSTALLOGRAPHY

While most people could not define crystallography, even young children readily recognize the word "crystal". Solids with distinct, shiny faces attract the admiration of almost everybody. Because of this, crystals are a great starting point for outreach to schools and the general public. This includes gemstone exhibits at museums, where crystallographers can volunteer to explain some of the crystal structures and how the symmetry of the unit cell affects the distinct shapes of many minerals, or discussions on how "impurity atoms" lend beauty (color) to crystals. The quartz family of minerals is especially well suited for this, as the interfacial angles are very characteristic and easily observed in most mineral specimens. In addition, quartz species are very reasonably priced, making it easy to acquire a small personal collection for outreach events. A set consisting of colorless quartz, purple amethyst, pink rose quartz, grey smoky quartz, and yellow-brown citrine works very well.

In addition to showing minerals and explaining the importance of both structure and atomic composition, few projects excite children and adults more than growing crystals themselves. Possible fast activities include "crystal gardens" grown in waterglass solution from common metal salts (growth within minutes), growth of lysozyme crystals as pioneered by the YSSIG (growth within hours) or the University of Tennessee's "crystal jars" that grow borax crystals on floss or pipe cleaners, which can be colored through addition of food coloring (growth within hours). Long term experiments may use alum or copper sulfate, and introduce concepts like using seed crystals to grow larger crystals from supersaturated solutions. This latter category also offers itself to crystal growing contests. While such contests have been common for a number of years in some countries, the United States are hosting their first national crystal growing contest during IYCr2014. Hopefully, such contests will become a permanent establishment and attract more students every year.

3. FUN WITH LIGHT – GETTING MORE SERIOUS ABOUT CRYSTALLOGRAPHY

As we all know, the diffraction of visible light by gratings follows similar laws as the diffraction of X-rays, neutrons or electrons by crystalline materials. While Bragg's law may be an oversimplification of what happens in a diffraction experiment, it works well for introducing middle or high school students to some basic concepts of crystallography. In addition, the use of lasers and gratings allows students of all ages to explore the reciprocal relationship between crystal space and diffraction space without apprehension about Fourier transforms or other complex math or physics concepts. We have found during the "Crystallography: A World of Wonders" workshop for school teachers that use of two slides from the *Institute of Chemical Education's* (ICE) original "Optical Transform Kit" work well to explain crystallographic diffraction experiments, and that this demonstration can be adapted to any age level. The Discovery Slide illustrates the nature of reciprocal space through sets of differently oriented and spaced lines and dots, giving 1D or 2D diffraction spot arrays with different spacings. Obviously, this can be related to the spacing and orientation of the lines or dots on the slide, and shows that the location of diffraction spots contains information about the periodicity of the diffracting object. The second slide we have used is the VSEPR slide, also called "Structure of triatomic molecules". While this slide has been discontinued, it can still be ordered by directly contacting

ICE if enough lead time is given. On this slide, all “unit cells” have the same size and thus give rise to diffraction spots in the same locations, but due to the different shape of the features, the intensities vary. This observation can be used to explain that the intensities of the diffraction spots contain information about the type and location of the atoms within the unit cell. In the future, we will explore with ICE whether it may be possible to design a single slide that would illustrate both of these concepts, which would reduce the funds needed for the purchase of outreach materials.

4. FUN WITH SYMMETRY – CRYSTALLOGRAPHY’S RELATIONSHIP WITH MATH AND ARTS

It is impossible to study crystallography without a thorough understanding of symmetry. However, crystallography does not hold a monopoly on symmetry, which is abundantly present in many other fields, most noticeably in math and art. This allows us to connect with these other subjects, to use art to illustrate symmetry concepts important in crystallography, and to explore whether crystallographic material can be incorporated into the Next Generation Science Standards. An example that demonstrates how symmetry can connect artists and crystallographers is the work of M.C. Escher, who was inspired by papers written by Haag and Pólya. Escher’s drawings still offer a great opportunity to attract the curiosity of the general public to crystallography related topics, which Doris Schattschneider proved during her public talk on “M.C. Escher and Crystallography” during the “World of Wonders” workshop at the 2014 ACA meeting.

5. SPECIFIC ACTIVITIES DURING IYCR2014

5.1. Website

Under the auspices of IUCr’s umbrella website iycr2014.org, the ACA has developed a website to summarize all outreach activities, contests, educational material and more. This site will be launched in the near future, and can be found at http://www.iycr2014.org/aca/home. A major purpose of this website is to serve as a repository for educational materials and historical knowledge, which is expected to provide a valuable resource far beyond the year 2014. The educational portion is subdivided into three categories, and features theoretical material and hands-on activities for Grade School, High School, and University level. Links to short educational videos on different topics are also provided. Submission of additional materials by all crystallographers and educators is strongly encouraged! Another fun feature of the website is “Crystal Connect”, which allows people to get connected with a close-by crystallographer to help organize talks or events.

5.2. Contests

As mentioned earlier, the United States are hosting their first crystal growing contest during IYCr2014. Rules were established with some friendly help from the Canadian neighbors, who have held crystal growing contests for about a decade. This contest will be open to students enrolled in K-12 grades, including homeschooled students. Alum, $KAl(SO_4)_2 \cdot 12H_2O$, will be available for free or a nominal fee thanks to sponsorship by Ward’s Science and the University of Buffalo Department of Chemistry. Crystals must be grown between October 20 and November 24, 2014, and weigh at least 0.5 g to be eligible to enter. Judging will take place in December, and will be divided into K-8 grade, 9-12 grade, and teacher crystals. For each student

category, cash prizes will be awarded both for best overall crystal and best quality crystal. Winning crystals will become part of a permanent display at SUNY Buffalo.
Regional or state level crystal growing contests are also underway, like the Wisconsin contest for high school students, which is underway in April and May. In this contest, copper sulfate pentahydrate, $CuSO_4 \cdot 5H_2O$, is used for crystal growth.
In a joint effort Canada and the United States will be hosting a North American video contest, which is open to K-12 students in both countries. Videos will be collected via a Facebook page, and can highlight crystallography experiments carried out by the students, the impact of a historical experiment on science or society, a famous scientist who used crystallography in their research, or math or physics concepts related to diffraction, structure determination, or symmetry. The site will be open for submissions from July 1 through December 31, 2014. Finalists will be selected based on the number of "likes", but a panel of experts will select the winning videos and award cash prizes in early 2015.

5.3. Highlighting Nobel Laureates

Nobel Laureates always attract the attention of the general public, and crystallographers have received a large number of Nobel Prizes. This provides a great approach for highlighting the contributions of crystallography through many different venues. A prominent example that reached a large number of people was Google's May 12, 2014 Doodle, which commemorated Dorothy Hodgkin's 104^{th} birthday and depicted the crystal structure of penicillin. This doodle was featured across North America, Colombia, the northern coast of Africa, Kenya, South Africa, most of the Arabic Peninsula, parts of Europe, India, Japan, South Korea, Taiwan, Malaysia, Indonesia, and the Philippines. Many IYCr websites and museum exhibits also prominently feature crystallography Nobel Laureates. Dorothy Hodgkin has been selected as a particularly appropriate person to highlight by the ACA, as she received the Nobel Prize 50 years ago, and passed away 20 years ago. Her example also highlights that crystallography has long been open to contributions by women.

5.4. Reaching out to other societies

All science and engineering disciplines have immensely benefited from crystallographic discoveries, as modern research largely focuses on structure-property relationships. This makes it appropriate to highlight the contributions of crystallography at meetings of other societies. Special symposia or sessions have been held at the American Chemical Society National Meeting in Dallas, the Biophysical Society Meeting in San Francisco, and The Minerals, Metals & Materials Society Meeting in San Diego.
In addition, the ACA has reached out to other organizations on an educational level. A number of ideas for this outreach stem from the "Crystallography: A World of Wonders" (CWOW) workshop, which was offered for school teachers at the 2010 Chicago and 2012 Boston ACA meetings. A third full-day CWOW workshop is held in conjunction with the 2014 Albuquerque meeting, however, in contrast to past workshops, this year's event is hosted off-site at the New Mexico Museum of Natural History and Science. The full workshop includes lectures on structure, diffraction basics, use of diffraction to analyze everyday materials, and CCDC and PDB. Hands-on exercises on materials matching games, Lego crystal structures, lasers and gratings, and use of databases complement the lectures. In addition to the full-fledged workshop, a shorter adaptation of CWOW, focusing on selected topics, have been introduced at the April

national meeting of the National Science Teacher Association (NSTA) in Boston. The best format for a presentation at a fall NSTA meeting is currently under exploration.
The Young Scientist SIG started a very successful outreach program at the 2012 Boston meeting, working with local high schools to carry out lysozyme crystallization experiments. Students were connected with local crystallographers for site visits to see how well their crystals diffracted. They presented their results in poster format at the ACA meeting. The Boston experiment was continued by at least one of the high school teachers, and the YSSIG has started new seed projects in Hawaii and Albuquerque in 2013 and 2014. This year, they also set up an *in situ* experiment to grow lysozyme crystals at the Albuquerque Museum of Natural History and Science to attract visitors to the public lecture on Escher and Crystallography.
The American Institute of Physics has created and assembled Science Outreach Catalyst Kits (SOCKs) for more than a decade. The 2014 kit will include crystal jars (borax crystal growth), diffraction demos, and symmetry related materials. The kits will be assembled over the summer, and will be available for Society of Physics Students chapters in the fall. The diffraction demo will be useful for discussing both IYCr2014 and the International Year of Light 2015.
The Geosciences Institute has announced that they will include crystallography experiments in their activities for Earth Science Week 2014.
IYCr will also be represented in the Teachers' Materials Camps run by the ASM Educational Foundation this year. ASM holds 40 1-week camps at a number of locations around the US during the summer, where groups of 25 high school and middle school teachers are taught the basics of Material Science. Teachers will be supplied with handouts on IYCr and important contributions of crystallography to science and engineering. They will also be made aware of the website and its collection of facts, videos, and hands-on activities.

5.5. Workshops and schools

Many crystallography related workshops and schools have been run annually for a number of years and are thus not specific to IYCr. A noteworthy special set of schools are the courses in powder and single crystal X-ray diffraction techniques that are jointly hosted by the Colombian and Venezuelan societies of crystallography, with an open invitation extended to crystallographers from across the Latin American countries. The powder workshop will be held in June in Mérida, Venezuela, and acknowledges support from the ICDD and UCNCCr to allow participation of specialized instructors residing in the US. The single crystal workshop will be held in September in Bucaramanga, Colombia.

5.6. Miscellaneous special events and activities

Canada is proud to host the IUCr meeting in Montréal during IYCr2014. In an effort to make crystallography accessible to the general public at the same time, Jean-Louis Hodeau's panels on "Voyage dans le cristal" (Journey into the Crystal) will be on display during the congress. In addition, a series of three public evening lectures on crystallography is planned.
During IYCr2014, the ACA joined forces with the ACS to present two webinars on crystallography. The first webinar on crystallography and everyday materials was broadcasted on May 15, with Robin Rogers as moderator and Cora Lind-Kovacs and Jim Kaduk as speakers. The webinar was well attended, and feedback by the audience was positive. Attendees included at least one participant of the 2010 CWOW workshop, showing that the initial interest sparked by such outreach activities can persist throughout the years. A second webinar on biological applications of crystallography is planned for October.

In a unique effort to bring crystallography to the general public, Matthew Dougherty has been seeking funding to create a planetarium show that illustrates point groups, crystals and gems. This approach automatically pulls in other scientific societies as well.

In Ohio, district leaders of the Girls Scouts have expressed interest in working with universities to create a flexible curriculum on crystallography. This curriculum will include adaptations for different age groups, and options for time commitments ranging from standalone sessions to six week curricula. This effort is spearheaded by the Alpha Chi Sigma fraternity at the University of Toledo, with short trial sessions planned for the next few months. The long term goal is to develop a detailed set of instructions that allows girl scout leaders to teach these sessions independently.

As part of the "Biggest Open House in Texas" at "Explore UT", Marvin Hackert presented an exhibit on "Crystals and Crystallography". His well-attended exhibit included posters, demonstrations and experiments, and covered topics like crystal growth, symmetry, optical transforms and atomic level structure. Traditionally constructed models and 3D printed models of a number of small and large molecules fascinated the audience.

The events described in this point are by no means an exclusive list, but we hope that they will give a flavor of the types of activities pursued by ACA members during IYCr2014. Once the website is fully functional, a much better overview of all events will be available.

6. LEAVING A LEGACY

The sections above are an attempt to summarize ways in which crystallographers can reach out and interact with society, students of all ages, or scientists and engineers who are less familiar with our science. In the current climate of limited federal research funding, reorganization of many aspects of higher education, and a gradual elimination of formal crystallography instruction from many curricula, it is crucial that we make as many people as possible aware of the tremendous impact that crystallography has had on modern science and engineering, and on many aspects of life in general. Failure to do so will result in further marginalization of our science, and could lead to stagnation or even significant loss of expertise. In recognition of this, the ACA has recently declared Outreach and Education as two of its four key objectives. Exposing students to some basic crystallographic concepts at a young age through incorporation into the Next Generation Science Standards, and attracting their curiosity through fun and thought-provoking activities, will ensure continued growth of "tomorrow's crystallographers". The websites created by the ACA and other affiliates have the potential to become an enduring legacy that experts and novices alike can visit to gain insights, connect with experts, or simply refresh their memory on some topics. But what we have to keep in mind is that *we* are the current experts who have to contribute the knowledge to this repository, that *we* are those crystallographers that site visitors may wish to connect with. Without our willingness to be the hands, feet and voice of crystallography, this legacy may remain hidden. We hope that this glimpse of outreach ideas will excite many to help put crystallography in the spotlight instead.

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