

## ■ 会議報告

# 23<sup>rd</sup> Congress and General Assembly of the International Union of Crystallography (IUCr2014) Report [Materials science field]

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If you are a grad student, a young researcher, or a scientist who wants to know the most recent advances in crystallography, I would recommend attending the Congress and General Assembly of the International Union of Crystallography. It is, to the best of my knowledge, the largest international meeting for people in many branches of science putting their heart and soul into crystallography (the branch of science devoted to the study of molecular and crystalline structure and properties, with far-reaching applications in mineralogy, chemistry, physics, mathematics, biology and materials science. <http://www.iucr.org/>). This meeting has been held every three years ever since the first one in Cambridge, Massachusetts in 1948, a year after the International Union of Crystallography was formed based on an idea proposed by Paul Peter Ewald in 1944. Japan has hosted the congress twice; one was in Kyoto in 1972 and the other in Osaka in 2008. The amount of new information presented during the congress is enormous and it is literally impossible to keep up with what has been going on in all fields of crystallography. Therefore, I mainly give a rough overview of what the congress is like in this report. I deeply apologize in advance for delivering science only limited to the field that I am involved in.

This year, the 23rd congress took place in Montreal, the second largest city in Canada, from August 5 to 12. This year's congress is very meaningful because the United Nations declared 2014 as the International Year of Crystallography to mark the centenary of a series of historic experiments by William Henry Bragg, William Lawrence Bragg (father and son) and Max von Laue which established the modern science of X-ray crystallography. This year is also the 400th anniversary of Kepler's observation of the symmetrical form of ice crystals (<http://www.iucr2014.org/>). Many events and activities celebrating the International Year of Crystallography are taking place all over the world.

The first day of the congress, as usual, was dedicated to a half or full day workshops for various structure determination techniques and software programs. I think this is a

perfect opportunity to learn new techniques or programs directly from experts or program developers. This year's workshops include introduction to aperiodic crystals, XAFS (X-ray Absorption Fine Structure), the USPEX code (Universal Structure Predictor: Evolutionary Xtallography) for crystal structure prediction, the SHELX program for small and macromolecular crystal structure determination, and OLEX2 program for structural solution and refinement. There was also a workshop for the utilization of XFEL (X-ray Free Electron Laser) facilities. In addition, various commission and council meetings took place throughout the congress period.

The congress officially began in the evening of the first day. At the opening ceremony, the presentation of the Ewald Prize was made. The Ewald Prize has been awarded every three years to outstanding contributors to the science of crystallography since 1986. This year's winner is Professors Aloysio Janner and Ted W. J. M. Janssen from the University of Nijmegen in the Netherlands for the development of superspace crystallography and its application to the analysis of aperiodic crystals. Prof. Janssen gave an Ewald Prize lecture. In addition to the Ewald Prize, the Gjønnnes Medal was also given to outstanding contributors to the field of electron crystallography. This year's recipients are Professor Michiyoshi Tanaka from Tohoku University in Japan and Professor John Steeds from the University of Bristol in England for their contributions to convergent-beam electron diffraction.

The scientific program scheduled from the second day of the congress was very rich. Each day started with three parallel keynote lectures followed by eight parallel microsymbiosia until late afternoon. At each microsymbiosium session three invited and three regular talks were given. The oral session was completed after three parallel keynote lectures and a plenary lecture in the late afternoon. In the evening, the poster sessions were held until 8 : 30 p.m. This year, there were one Ewald Prize, two Gjønnnes Prize, four plenary and 34 keynote lectures. Total 112 microsymbiosia covering a wide range of topics were or-



**Prof. Greedan from McMaster University in Canada talking about magnetic ordering in double perovskites.**

ganized and around 1300 posters were presented. In addition, software fayre, where developers of open-source software programs demonstrate their software programs with some practical examples, took place concurrently with microsymposia. Industrial workshops were held during lunch time sometimes providing free lunch. Of course, all work and no play makes Jack a dull boy. Several social activities like tours, Jazz Night, and Banquet were arranged for the congress participants and accompanying persons to learn and enjoy the beautiful and vibrant city of Montreal.

The amount of new science I encountered during the congress was overwhelming. The total scattering community that I am mainly involved in has grown considerably for past three years. There were certainly an increasing number of oral and poster presentations covering this topic compared to the last congress. In particular, a large number of studies were dedicated to observation of how nanoparticles grow by in situ time resolved total scattering experiments. This experiment utilizing high flux and high energy synchrotron X-ray and a fast-readout area detector was first carried out by Peter J. Chupas and his colleagues at the Advanced Photon Source (APS) in the U.S. seven years ago and now similar experiments can be conducted in various other synchrotron facilities. Another popular topic was Li-ion battery material. Karena W. Chapman at the APS has developed in situ operando total scattering setup



**A mix of modern and historic buildings creates a captivating landscape in Montreal.**

to investigate local structural change in Li-ion battery materials during charging and discharging processes. Several successful examples using this setup were presented. Reinhard B. Neder from the University of Erlangen-Nürnberg in Germany showed a possible way to handle the effect of preferred orientation in the atomic pair distribution function. The complex modeling approach, in which multiple experimental inputs and theoretical constraints are combined to optimize a structural model, seems to be the mainstream of the software development in the total scattering field and there are already several successful studies available. My greatest reward of this year's congress was an encounter with ISODISTORT, a software allowing us to generate and explore the structural distortion modes of crystalline materials. This software has tremendous potential to unlock local distortions in various crystalline materials.

The congress becomes more and more exciting each time. It provides many opportunities to make new friends and to encounter interesting new science. The next congress will be held in Hyderabad, India in 2017. I hope this report encourages you to give it a try.