

Triennial Report 2005 – 2007 of the IUCr Commission on High Pressure.

As usual for new trienniums, the Commission on High Pressure started its fourth triennium in a new composition. Four very active members (John Parise (US), Russ Hemley (US), Werner Kuhs (D), Igor Goncharenko (F)) reached the limit of their terms and were replaced by Vladimir Soloshenko (F), Simon Redfern (UK), Andrzej Katrusiak (Po) and Giulia Galli (US). With these new members the commission consisted of the following members for the past 3 years:

Martin Kunz (CH, now USA, male, Chair)

John Tse (Can, male, Treasurer)

John Loveday (UK, male, Secretary)

Sarah Tolbert (USA, female)

Giulia Galli (USA, female)

Roland Winter (D, male)

Nom Hamaya (Japan, male)

Mohamed Mezouar (F, male)

Andrzej Katrusiak (Po, male)

Simon Redfern (UK, male)

Vladimir Solozhenko (F, male)

The commission furthermore benefitted from the advice of the following consultants:

Richard Nelmes (UK), Igor Goncharenko (F), Przemek Dera (USA), Guoyin Shen (USA), Ross Angel (USA).

The unusual size of the commission (10 members plus the chair) is essential to maintain competent expertise throughout the broad range of different scientific topics covered by the interdisciplinary field of high-pressure crystallography.

The past triennium was marked by the tragic and unexpected passing of Commission consultant Igor Goncharenko in a scuba diving accident. The commission lost an exceptionally active and supportive member and the high-pressure crystallography community lost an outstanding scientist among its ranks. Igor was nominated as a key note lecturer for the upcoming IUCr congress.

The past three years brought a range of new development in high pressure crystallography, but also a consolidation of high-pressure as a technique to explore the interdependence

between structure and properties in condensed materials. One of the exciting new developments in the past three years is the more and more sophisticated exploration of amorphous and liquid structures at high pressure. Also, the simultaneous combination of neutron and/or X-ray scattering techniques with other probes, such as e.g. Brillouin spectroscopy or transport property measurements allows a very accurate correlation of structure and property with pressure and temperature as variable parameters. New developments at neutron and synchrotron sources continue to play an important role in these improvements, as much as successful programs at small research groups across the world. The recognition of the importance of complementary experiments to obtain a comprehensive picture of the interdependence of structure and properties lead to an increase in coordinated collaborations between different techniques. A prominent example is the formal establishment of the High Pressure Synergetic Consortium, HPSynC at the APS.

The past three years have also seen a renewed interest in 'old' techniques such as high-pressure single crystal diffraction, which we find more and more moving from its established place in small university labs to large scale facilities, such as synchrotrons (ESRF, APS, Spring-8) and neutron sources (ISIS, SNS). This enables the expansion of accurate crystallography to higher pressures and temperature.

The role adopted by the IUCr Commission for High Pressure in this dynamic field is to facilitate and enable the exchange of new ideas and developments at as early a stage as possible. Also, the commission is dedicated to help connecting talented young researchers with established and experienced high-pressure crystallographers. This is not only to help the young people with their research problems, but also for the benefit of the high-pressure community in that it helps grow new ideas from fresh minds.

The main tools available to the Commission for High-Pressure Crystallography to achieve this goal are annual workshops on high-pressure crystallography. Also, the Commission helps shaping a strong high-pressure program at the triennial General Congress of the IUCr. In addition, commission members and consultants are heavily involved in organizing a variety of summer schools dedicated to high-pressure crystallography (e.g. Erice 2003, Isle of Skye 2008, Erice 2009).

Symposia and workshops:

During the XX IUCr General Congress and Assembly, the commission organized 6 microsymbosia. The topics covered were 'biological and organic soft condensed material under pressure', 'computational crystallography applied to extreme conditions', 'novel materials under high pressure', 'structural phase transitions and properties at high pressure', 'crystallography at conditions of earth and planetary interiors', and 'liquids and amorphous

systems at high pressure'. In addition, commission members John Loveday and Igor Goncharenko organized two open commission meetings on the topics on 'technical development in high-pressure crystallography' on one hand and 'advances in high-pressure single-crystal diffraction' on the other hand. Both, microsymbosia and open commission meetings (OCM) were very well attended with attendances between 60 (OCM's) and 100 (microsymposia) persons.

The commission was also happy to see two of the keynote lectures to be given by high-pressure scientists, namely Dr. John Tse (CLS, commission member) and Dr. Malcolm Mc Mahon (Univ. Edinburgh).

The commission makes a conscious effort to be as internationally inclusive as possible. For this reason a workshop was held in Russia in 2006, and next year's workshop is planned in China:

The International Workshop on Crystallography at High Pressure 2006 followed the sequence of workshops organized on behalf of the IUCr Commission on High Pressure and also the sequence of meetings on Neutron Scattering at High Pressure organized by the FLNP JINR (NSHP-I in 1994 and NSHP-II in 1999, Dubna, Russia). It was organized at the Frank Laboratory of Neutron Physics and Joint Institute for Nuclear Research in Dubna, Russia from September 28 through October 1, 2006. The organization was coordinated by Denis P. Kozlenko. Igor Goncharenko served as the liaison to the commission.

The Workshop attracted nearly 80 scientists from 10 countries. Its scientific program contained 10 oral sessions and 2 poster sessions, covering the full range of scientific activities of the Commission on High Pressure.

The 2007 workshop was held between September 3rd and September 7th at Wadham College in Oxford, UK. Commission Secretary John Loveday acted as the local organizer. This workshop was again a big success. 85 participants gathered in a historic music pavilion to follow 11 oral sessions and poster presentations. The workshop was finished with a tour through the new synchrotron facility (Diamond) and the highly successful ISIS neutron spallation source at Ruherford Appleton Laboratory.

Presently, the Commission's focus is on helping to shape an attractive high-pressure program within the XXI IUCr congress in Osaka. Nom Hamaya acts as the Commission's representative in the program committee. The commission is able to organize 6 microsymbosia (two of which joined with the Commission for Chemical Crystallography and Commission for Inorganic Materials and Minerals, respectively). Furthermore, 2 candidates proposed by the Commission for high-pressure were accepted as keynote speakers (Giulia

Galli and Igor Goncharenko). Due to Igor's tragic death, his keynote slot was filled with Stefan Klotz (F).

Commission Meetings

The commission held a meeting during the 2006 high-pressure workshop. 7 commission members were present. One of the most important topics discussed was the replacement of expiring commission members in 2008. Further points of discussion were the high-pressure program of the upcoming IUCr congress in Osaka, as well as an alternative and more reliable way of maintaining the commission's web-page.

Future Plans and activities:

The Commission plans more of its workshops in the years 2009 and 2010. In order to facilitate scientific exchange with the Chinese high-pressure crystallography community, it was decided to organize the 2009 workshop in Harbin (Heilongjiang Province, NE China). Commission consultant Przemek Dera is co-organizer of the 2009 edition of a summer school for high-pressure crystallography in Erice.

The venue of the 2010 workshop has not been not decided yet.

Martin Kunz, Berkeley, May 6th, 2008