

From June 4 - 14, 2009 one hundred twenty two total participants convened at the E. Majorana Centre for Scientific Culture, Erice, Italy for the 41st Course of the "International School of Crystallography", one of more than a hundred cultural sections of the Centre.

General information

This was the second course dedicated to high-pressure research, which followed the very successful first course, organized in 2003 by A. Katrusiak and P. McMillan. The course of 2009 was co-directed by Elena Boldyreva (Novosibirsk, Russia) and Przemek Dera (Chicago, USA) and was supported by the IUCr Commissions on High-Pressure, Teaching, Inorganic and Mineral Structures. As usual, the team or local organizers was very professionally led by Lodovico Riva di Sanseverino (Bologna, Italy) and Paola Spadon (Padova, Italy). The “orange scarfs” did a great job of organizing the Meeting. As one of the participants has written in the post-meeting questionnaire: “All we, participants, had to do, was to be on time. The organizers did the rest of the job”.

The School was sponsored by IUCr, ECA, University of Bologna, and supported by ICDD, Compres, Psi-k, Almax-Industries, Bruker, Crystal Impact, D’anvils, Oxford Diffraction (now part of Varian) and STOE. NSF (USA) and RFBR (Russia) supported financially the participants from the USA and Russia, respectively. Many lecturers acted as “private sponsors”, having generously agreed to cover their travel expenses, and, partly or totally the participation fee for their students, from their own research funds, and in some cases, even using their private money, what is very much appreciated. At the very last moment (two days before the School started!) the application for NATO grant from the Science for Peace and Security program was approved. The unfortunate delay in receiving the grant approval resulted in few withdrawals by some applicants in need of support and unable to buy the flight-tickets within the uncertain atmosphere. Nevertheless, a substantial number of students in need of support were able to come on the assurance by the optimistic attitude of the organizing committee, and there was indeed a flow of reimbursements to those who had risked on the organizers’ assurance that a support would any way be found. The scientific planning and follow-up did not suffer for the above mentioned delay and the foreseen program was brought forward successfully.

The country distribution reflected the existing situation in the high-pressure science, with obvious domination by the USA, UK, Germany, France, Italy, Russia, Poland, and Spain, but also many other countries represented (Sweden, China, India, Netherlands, South Africa, Israel, Switzerland, Belarus, Nigeria, Ukraine, Czech, Colombia, Brazil, Portugal). Asian, South-American and African countries have been obviously under-represented, but this was related first of all to the lack of funding for these participants, all of the applicants requesting a complete financial support. As the experience of Poland, Russia, and USA has shown, the availability of funding from local (national) sponsors plays a decisive role in increasing the attendance from a country. For example, 10 fellowships have been provided by the NSF and COMPRES, to support the participation of the American students in the school.

The gender distribution of speakers and participants was still far from the “ideal” 50% to 50% , but there have been noticeable improvements as compared with the past: 8 out of 46 speakers, and 44 out of 122 participants were females. Age distribution among the lecturers have also shifted towards younger age: 66 % of speakers were younger than 50 years old. A novel feature of an Erice crystallography school in 2009 was that a “young participant” did not necessarily mean “a young participant presenting / not presenting a poster. 20% of invited speakers were younger than 35 years old, that is they could be qualified as “young participants” (Nicola Casati, Italy; Olga Degtyareva, UK; Francesca Fabbiani, Germany; Jaroslav Filinchuk, France; Diego

Gatta, Italy; Jeniffer Jackson, USA; Denis Kozlenko, Russia; Sebastien Merkel, France; Artem Oganov, USA). The youngest lecturer (Francesca Fabbiani, Germany, 29 years old) was only a few years older than the youngest participants presenting posters (Wanaruk Chaimayo, UK and Vasil Minkov, Russia, 23 years old). Despite their young age, these speakers have done an exceptionally good job, and their lectures were mature, educational and very well-presented.

Scientific agenda

As a thermodynamic parameter, pressure is remarkable in many ways. It spans in the visible universe over sixty orders of magnitude, from the non-equilibrium pressure of hydrogen in intergalactic space, to the kind of pressure encountered within neutron stars. In the laboratory, it provides unique possibility to control structure and properties of materials, dramatically alter electronic properties, break existing, or form new chemical bonds by reaching compressions in excess of an order of magnitude for molecular materials.

This agenda naturally encompasses elements of physics (properties and structure), chemistry (chemical reactions, transport), materials science (new materials) and engineering (mechanical properties); in addition it has direct applications and implications for geology (minerals in their natural, deep earth environments), planetary sciences, biology and medicine (deep sea ecosystems, membranes, protein and nucleic acid folding, the role of high-pressure in the origin of prebiotic forms of matter and the origin of life, deactivation of viruses and toxins).

Beyond its specificity, high-pressure science finds direct or indirect (i.e. economic) application in several fields of modern technology, such as mechanical engineering (strain/stress analysis), optoelectronics and spintronics, nanotechnology, pharmaceutical industry, food processing, petroleum industry, seismic data interpretation, etc.

Lectures

Such a variety of topics, explains a very “densely packed” program, which have “kept the participants under pressure” during the 10 days. 56 lectures were given by 46 speakers.

The school started with a general introduction into high-pressure science given by P. Dera (USA). M. Paz-Pasternak (Israel) spoke about the principles of operation of the diamond anvil cells and on the most modern trends in their development. Yanbin Wang (USA) gave a comprehensive introduction into the large volume press techniques. M. Mezouar (France) and P. Dera (USA) described the different flavors of synchrotron X-ray diffraction at high pressure, including the high- and low-temperature research. Jennifer Jackson (USA) spoke on synchrotron- based spectroscopic techniques, including Mossbauer and high-resolution inelastic scattering. J.-P. Itie (France) gave an introduction into X-ray absorption spectroscopy. Leonid Dubrovinsky (Germany) discussed different approaches to measuring the transport properties under pressure. Sebastien Merkel (France) and Yanbin Wang (USA) considered the experimental study of plastic properties, texture analysis, elasticity, plasticity and rheology of minerals and materials. Anatoly Balagurov (Russia) and John Loveday (UK) gave a comprehensive introduction into the present day high-intensity and high-resolution neutron diffraction and neutron scattering at high pressure. Apart of these lectures specially focused on the techniques, other lectures devoted to the phenomena also illustrated the applications of various experimental techniques and approaches.

Considering phenomena started with the “simplest” possible one: compression without any phase transitions or chemical transformations. Tiziana Boffa-Ballaran (Germany) discussed the basics of the calculation of the equation of states from the experimental data and its application in

geosciences. Robert T. Downs (USA) gave a beautiful introduction into the compression systematics in minerals, focusing on the anisotropy of strain and the interrelation between the structures and the properties. This lecture was followed by an introduction into the compressibility of molecular crystals given by Elena Boldyreva (Russia), who showed, what kind of knowledge about the intermolecular interactions in these systems can be gained from studying the strain anisotropy. The lectures by Downs and Boldyreva demonstrated, how much similarity one can find in the structural response of inorganic and organic systems to pressure, if interatomic interactions are considered. The topic of using pressure as a tool for studying the intermolecular interactions was continued by Andrzej Katrusiak (Poland), who has considered pressure-induced crystallization of liquids, Nicola Casati (Italy), who discussed the effects of high pressure on the intra-molecular geometry, and Bjorn Winkler (Germany), who spoke on the experimental and modeling studies of the role of hydrogen bonding in minerals at high pressure. Piero Macchi (Switzerland) gave a comprehensive introduction into the semi-empirical & ab initio quantum chemistry description of solid state phases under high pressures with a special emphasis on the systems with hydrogen bonds, stacking interactions, etc. – i.e. on organic and organometallic systems.

Phase transitions induced by high-pressure have been considered in details in another block of lectures, including both theoretical and experimental research. Vladimir Dmitriev (France) made a general introduction into the theory of phase transitions, Heidrun Sowa (Germany) spoke on the symmetry aspects in AB systems. Several lectures have been devoted to phase transitions in materials: Moshe Paz-Pasternak (Israel) discussed the crystallographic structural responses to pressure-induced electronic-magnetic transitions, Denis Kozlenko (Russia) considered physical phenomena in strongly correlated magnetic oxides and the lessons one can learn from neutron diffraction at high pressures, Andrzej Katrusiak (Poland) discussed phase transitions in hydrogen-bonded organic crystals – molecular materials, Fernando Rodriguez (Spain) gave an introduction into the Jahn-Teller systems at high pressure, J.-P. Itie (France) discussed the local aspects of high-pressure transitions in ferroelectrics. Phase transitions in crystalline amino acids and the information, one can gain from a combination of X-ray diffraction and Raman spectroscopy techniques, were considered by Paulo Freire (Brazil). Phase transitions in relation to earth sciences were discussed by Jennifer Jackson (USA) in relation with seismic activity, and by Leonid Dubrovinsky (Germany), who reviewed the effects of spin transitions in iron on the structure and properties of Mantle minerals.

High-pressure structures and properties of various types of solids, formed by “simple” elements or small molecules were covered in another lecture block. This block started with an introduction into high-pressure research of hydrogen and hydrides, presented by Florent Occelli (France). This topic was originally allocated to Igor Goncharenko, a recognized world leader in the field, who disappeared in a diving accident in 2007, and the lecture started with paying tribute to him and his work. Mario Santoro (Italy) spoke about carbon dioxide, Alain Polian (France) – about boron and boron-rich solids, Yaroslav Filinchuk (France) – about light metal borohydrides. Olga Degtyareva (UK) gave a comprehensive overview of the effect of pressure on the structures of metals, showing the beauty and the complexity of this field. Igor Abrikosov (Sweden) gave a lecture on the first principles simulations of alloy thermodynamics in megabar pressure range, and Sandro Scandolo (Italy) considered the first-principles molecular dynamics of small-molecule systems in relation to planetary science. In a special evening lecture Wojciech Grochala (Poland) demonstrated, how a MO approach can help to interpret high-pressure phenomena from a “chemical point of view”, using the synthesis of AuF as an example.

The lecture block related to the structures of materials at high-pressures was opened by a comprehensive overview on high-pressure synthesis of advanced materials presented by Paul McMillan (UK). Jens Kreisel (France) considered the effect of high-pressure on functional

dielectric perovskite-type oxides, Diego Gatta (Italy) illustrated, that the microporous materials at high-pressure are not really soft, and gave examples of pressure-induced expansion due to incorporation of liquids or gasses into the cavities, Colin Pulham (UK) introduced the audience into the fascinating field of the energetic materials (explosives), using the most advanced audio and video effects. Andrea Gauzzi (France) spoke on high pressure & superconductivity, using intercalated graphite CaC_{66} as a model system, Vladimir Solozhenko (France) gave a comprehensive overview of the state of art in the high-pressure synthesis of novel superhard phases in the B-C-N-O system, Bjorn Winkler (Germany) considered the synthesis and structure-property relations of binary metal carbides studied in laser heated diamond anvil cells and with density functional theory calculations, Alfonso San Miguel (France) discussed the applications of Raman spectroscopy to studying carbon nanotubes at high pressure. Artem Oganov (USA) gave an introduction into the theoretical prediction of high-pressure structures of minerals and materials, based, in particular, on using his software package USPEX. Crystelle Sanloup (UK) made an introduction into the field of amorphous materials at high pressure, and Paul McMillan (UK) discussed X-ray scattering approach to studying polyamorphic materials and amyloid fibrils. The nanomaterials at high pressures were discussed in the lecture given by Giovanni Hearne (South Africa), as well as in the lectures by John Parise (USA) and Lars Ehm (USA), devoted to the analysis of the total scattering using the quantitative HP pair distribution function.

The last but not least was a block of lectures on the materials and systems of biological importance, including the pharmaceuticals. An introductory lecture to this block was given by Elena Boldyreva (Russia). Francesca Fabbiani (Germany) gave an overview of the high-pressure crystallization of pharmaceuticals, as was already mentioned when considering the lecture block on phase transitions, Paulo Freire (Brazil) considered the effect of pressure on the crystalline amino acids. Roland Winter (Germany) revealed to the participants the “landscape” of biomolecules under extreme high-pressure conditions from lipid membranes to proteins, and Roger Fourme (France) described both the technical aspects and the recent achievements of the high-pressure crystallography.

Workshops and a round-table discussion

Five workshops and a round-table discussion were an important part of the school schedule. The first workshop was organized and led by Colin Pulham (UK) assisted by Kamil Dziubek (Poland) and Giovanni Hearne (South Africa). They showed at the podium, how to adjust a DAC, load a sample into the DAC and crystallize a liquid in it. Special thanks go to Colin, who brought all the equipment necessary for the demonstrations with him. Of course, this was just a very brief introduction – the only thing that we could afford, taking into account the limitations imposed by being at the Ettore Majorana Center, and not at a university lab. The second workshop was given by Yaroslav Filinchuk (France), who demonstrated, how to treat high-pressure X-ray diffraction data. Tiziana Boffa-Balaran (Germany) taught the participants, how to obtain reliable and correct data on the equation of state. Two further workshops given by Artem Oganov (USA) and Piero Macchi (Switzerland) were devoted to theoretical calculations of crystal structures and properties at high pressures using different algorithms. The approach described by Oganov is better applicable to inorganic systems, whereas that presented by Macchi is working well when dealing with organic, organometallic, coordination compounds. All the workshops were given as follow-me workshops, but hands-outs with detailed explanations were available, and the participants had an option to try using the software themselves after these introductory workshops, using the numerous computers available at the Ettore Majorana Center, as well as their own laptops.

The round-table discussion on the improvement of data collecting and processing in high-pressure single-crystal diffraction experiments was originally organized by Nicola Casati (Italy) assisted by Francesca Fabbiani (Germany), Kamil Dziubek (Poland), Przemek Dera (USA), Diego Gatta (Italy), Andrzej Katrusiak (Poland). Many more people have made valuable comments and suggestions (Mohamed Mezour (France), Roger Fourme (France), Tiziana Boffa-Balaran (Germany), Robert Downs (USA), Yaroslav Filinchuk (France), Michael Probert (UK), to list just a few). The “formal” round-table discussion has been followed by numerous smaller “Marsala room” and “breakfast room” discussions, which resulted in creating a set of three new online resources for the high-pressure crystallography community, which have been called Digital Resources for High Pressure Crystallography (DigResHPX). The DigResHPX package includes: High Pressure Crystallography blog: <http://hpdac.net/>, High Pressure Crystallography mailing list: hpdac@hpc.amu.edu.pl, and High Pressure Crystallography wiki: <http://cars9.uchicago.edu/surfacewiki/HPCrystallography>. These online tools and services are meant to provide a communication platform for exchange of technical information, advice, references, discussions etc. relevant for high-pressure crystallography community. Similar resources (e.g. CCP4 wiki <http://ccp4wiki.org/~ccp4wiki/wiki/>) are already available to or being created by other specialized branches of crystallography. The success of these resources will, to a large extent, depend on how widely they will be used by a general community. The links to the resources are being made from the IUCr, Compres, EHPRG, AIRAPT, and other relevant sites.

Poster session

This year the time allocated for the poster session was doubled as compared with the previous schools: in addition to the traditional “Pasta” and “Pizza” evening sessions there were two “Lunch while watching” sessions, which combined beautiful food of Lodovico’s choice with the possibility to watch and discuss the posters in the open air of San Francesco court. The poster sessions were preceded by short oral presentations of all the posters given by the participants. The total number of posters presented was equal to 52, that is a little bit more than 60 % of “non-speaking” participants have used the option to participate in the school in an active mode. Among poster presenters there have been not just the young beginners, but also a world-recognized experts like Valentina Degtyareva (Russia), Malcolm McMahon (UK), Thomas Hansen (France), and others. This has greatly enhanced the general level of the presented posters and, at the same time, made it quite difficult to select an obvious leader for a “poster prize”. After some discussions, the organizers decided that it would be better to acknowledge the contributions of the young lecturers, and young workshop leaders, who have been pre-selected among the young participants based on the submitted abstracts and the recommendation letters.

Activity of young participants in the lecture hall

The activity of the participants in the lecture hall was high enough, as usual increasing steadily to the end of the School. The most active young participants asking very interesting questions were those, who have been also actively involved in preparing the school – i.e., the young invited speakers or workshop leaders (Artem Oganov, Olga Degtyareva, Francesca Fabbiani, Kamil Dziubek, Jeniffer Jackson, Nicola Casati, etc.). Among “non-speaking” active young participants one could name Michael Probert (UK), Susannah Dorfman (USA), Charlen Estrada (USA), Geertie Ganskow (Germany), Nasir Abbas (UK), Armand Budzianowski (Poland), Angelika Rosa (Switzerland), to list just a few.

The virtual course

This year the tradition of virtual course has been continued thanks to the enormous efforts of John Irwin (USA), Kamil Dziubek and Armand Budzianowski (Poland). The lectures have been

broadcasted to several countries. The largest audience of the virtual participants (30 people) was following the lectures in Novosibirsk despite a 5 hours time difference. This has been made possible thanks to a cooperation of the JointLab (Director Andrzej Arzhannikov) and REC-008 (Director Vladimir Boldyrev) of the Novosibirsk State University. Technical support of Nikolay Zanin (Centre of the New Information Technologies NSU), and the organizational efforts of Anna Nartova (REC-008) are gratefully acknowledged.

Most of the lecturers have kindly agreed to make their lectures available to public, and these versions can be downloaded from the HPCrystallography wiki (see DigResHPX above).

Course proceedings as a published book

A book with the lectures presented at the school is being prepared, to be published as part of the NATO Science for Peace and Security Series: B – Physics and Biophysics by Springer publishing company. The book is expected to be available by mid 2010.

Leisure and informal communication

As usual, the very intensive training at the lecture hall was interrupted twice by half-day excursions to Mozia, Selinunte and Segesta, as well as optional beach stays, which helped the participants to relax and to survive. These excursions, as well as long coffee-breaks, joint breakfasts, lunches and dinners, “Marsala room” sessions served well for mixing the participants at all the levels (including countries and ages mixing), and stimulated many informal discussions. As most of the participants have written in their answers to the post-meeting questionnaire, the opportunity to meet the experts and to communicate with them has been the priority number one when applying for the participation. This is why it is so important, that the lecturers stay in Erice during all the school term, and the organizers would like to thank once again everyone, who has followed this rule despite being very busy.