PREFACE

Figure 1. Audience, including local organizers (orange scarfs) and student participants during one of the lectures.

This volume is a collection of lectures presented during the 2009 International School on High-pressure Crystallography, which took place at the Ettore Majorana Center for Scientific Culture, between June 4 and 14, 2009, in the very picturesque Sicilian town of Erice. The 2009 school was the 41st course of the "International School of Crystallography" organized at the Majorana Center and was directed by Elena Boldyreva (Novosibirsk University) and Przemyslaw Dera (University of Chicago). Unmatched support and excellent on-site organization was provided by the expert team consisting of Prof. Paola Spadon (Uniersity of Padova), Prof. Lodovico Riva di San Severino (University of Bologna), Elena Papinutto and Prof. John Irvin (University of California, San Franciso), aided by great team of young local organizers ("orange scarfs").

Major part of funding for the school was provided by a grant from the NATO Science for Peace and Security program, through which the 2009 Erice school was recognized as a NATO Advanced Study Institute (ASI). The theme of the Erice ASI was "High-pressure Crystallography: Advanced Armor Materials and Protection from Explosives." Additional financial support for the event was provided by the United States National Science Foundation EAR Geophysics Program, Consortium for Materials Properties Research in Earth Sciences, International Union of Crystallography, European Crystallographic Association, International Center for Diffraction Data, Psi-kappa, and several industrial sponsors, including (in alphabetic order) Almax Industries, Bruker AXS, Crystal Impact, D'Anvils, Oxford Diffraction and Stoe.

Figure 2. Marsala social evening.

The 2009 Erice school was very well attended, with 122 participants including 46 lecturers and 76

student participants (undergraduate, graduate and post-graduate), and included 10 days of intensive study, hands-on instruction and panel discussions.

The meeting agenda included a unique blend of topics and disciplines that are never found covered at a single event. The format of school with emphasis on education, rather, than review of recent accomplishments allowed all attendees, both students, as well as lectures, to significantly broaden their perception of the synergy of the multidisciplinary facets of high-pressure science and its applications in everyday life, technology and security. In addition to 45-minute lecture presentations, the school offered several excellent and widely attended hands-on and follow-me workshops, which allowed the student participants to learn many advanced tricks of the trade from the top experts in the field.

The topics covered by the lectures focused on several important aspects of high-pressure science: physics (properties and structure), chemistry (chemical reactions, transport), materials science (new materials) and engineering (mechanical properties); implications for geology, geophysics and planetary science (minerals in their natural, deep earth environments), biology and medicine. In addition, direct or indirect (e.g. economic) applications of the high-pressure science in several fields of modern technology have been considered. Such a variety of topics, explains a very "densely packed" program, which "kept the participants under pressure" during the 10 days.

The contents of this book are organized in six rough thematic blocks: (A) Experimental techniques and introduction to fundamental phenomena and their description, (B) Superhard materials and materials science (C) Computational approaches in high-pressure science (D) Geophysics and high-pressure transformations of minerals and rocks, (E) Molecular materials and explosives under high stress, (F) High-pressure effects on biomimetics and biological matter.

The first theme introduces the most modern experimental techniques used to generate high-pressure and temperature conditions, as well as study the behavior of samples at these conditions. Special emphasis is placed on experimental methods used in mineral physics research.

Several excellent chapters review the field of hard and superhard materials with potential technological applications. Synthetic routes in terms of chemistry, technical approaches to the synthesis at extreme conditions (e.g., using diamond anvil cell, large volume press, or novel detonation techniques), both ex-situ and in-situ methods of characterization of the structure and properties of the novel materials are presented.

Figure 3. Panel discussion of software for high-pressure crystallography.

Several expert lecturers reviewed computational approaches to predicting structures and properties of materials at high pressure as well as designing new materials with specific properties.

Another large block of presentations deals with the issues of geophysical applications of high-pressure experiments and starts with a general introduction to the issue of phase transitions in the deep earth and their relation to seismic phenomena and seismic observations. Other general topics discussed include possibilities and mechanisms of incorporation of water into rock-forming minerals (e.g. during the process of subduction) and its consequences for seismically active areas, the phenomenon and consequences of spin transitions that occur in iron-containing minerals present in the Earth's lower mantle, as well as general trends in the structural transformations in upper mantle minerals. The geophysics session concludes with the discussion of the important issue of plastic deformation, defect formation and texture development in rocks and minerals.

Also, a large and very exciting segment of presentations is focused on the behavior of molecular materials at extreme conditions, many with significant relevance for planetary science. Problems such as in-situ crystallization at high-pressure, solvothermal crystallization, polymorphism control, hydrogen bond transformations, and conformational transformations were introduced.

Figure 4. Hands-on workshop on in-situ crystallization.

The final theme of the book is biological matter and biomimetics at extreme conditions, including environmental and geobiological aspects, deep-sea environments, habitability limits, as well as deactivation of viruses and bacteria.

Majority of the multimedia presentations shown at the Erice ASI are available online at:

http://cars9.uchicago.edu/surfacewiki/HPCrystallography/Erice2009/LecturePresentations

An important outcome of the "round table" discussion on data processing software was the birth of a set of three new online resources for the high-pressure crystallography community: Digital Resources for High Pressure Crystallography (DigResHPX). The DigResHPX package includes:

1. High Pressure Crystallography blog:
   http://hpdac.net/
2. High Pressure Crystallography mailing list:
   hpdac@hpc.amu.edu.pl
3. 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.

This book is the final fruit of the Erice ASI, and with it we are hoping to provide current and future students and researchers in high-pressure field with a valuable and unique reference that offers both background information, as well as an overview of the numerous facets of the modern high-pressure science and technology.

Finally, we would like to express our sincere thanks to all that helped make the 2009 Erice ASI happen: the sponsors, local organizers, lecturers and student participants – you all contributed to the success of the school and to this book! We also gratefully acknowledge the most valuable technical assistance in preparing the manuscript for the publication by our colleagues at home institutions: Nancy Lazarz in Chicago, Elena Achkasova, Antonina Polyakova and Vasily Minkov in Novosibirsk.

School directors,

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