The International School of Crystallography, 41st Course

D'anvils

COMPRES

ALMAX INDUSTRIES
supplier of diamond anvils - www.almax-industries.com

UCSF
University of California
San Francisco

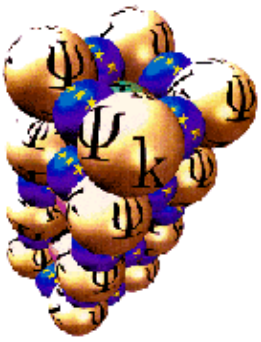
BRUKER ADVANCED X-RAY SOLUTIONS

BRUKER axs

CRYSTAL IMPACT

STOE

ICDD®



oxford diffraction

Now a part of Varian, Inc.

Programme for High Pressure Crystallography etc. (version June 03, 2009)

Erice, Italy: June 4 (**arrival day**) to June 14 (**departure day**), 2009

	June 5, Friday	June 6, Saturday	June 7, Sunday	June 8, Monday	June 9, Tuesday	June 10, Wednesday	June 11, Thursday	June 12, Friday	June 13, Saturday
8.45	**Paola Spadon** **Welcome**								
9.00 – 9.45	**Przemek Dera** Introduction to high pressure science	**Tiziana Boffa-Ballaran** Compressibility, EOS – applications in geosciences	**Florent Occelli** Hydrogen and hydrides at very high pressure. New approaches and recent results	**Sandro Scandolo** First-principles molecular dynamics and applications in planetary science	**Moshe Paz-Pasternak** Crystallographic Structural Responses to Pressure Induced Electronic-Magnetic Transitions	**Andrzej Katrusiak** Phase transitions in hydrogen-bonded organic crystal	**Elena Boldyreva** High-pressure studies of pharmaceuticals & biomimetics. Fundamentals and applications. A general introduction	**Roland Winter -** Exploring the "Landscape" of Biomolecules under Extreme HP Conditions: From Lipid Membranes to Proteins	**Andrea Gauzzi** High Pressure & superconductivity: intercalated graphite CaC_{66} as a model system
9.45 – 10.30	**Moshe Paz-Pasternak** Diamond anvil cell: principles of operation and most modern trends	**Robert T. Downs** Compression systematics in minerals	**Mario Santoro** Carbon dioxide at high pressure	**Artem Oganov** Theoretical prediction of HP structures	**Denis Kozlenko** Physical phenomena in strongly correlated magnetic oxides: lessons from neutron diffraction at H.P.	**Bjorn Winkler** Experimental and modelling studies of the role of hydrogen bonding in minerals at high pressure	**Francesca Fabbiani** New frontiers in physical form discovery: high-pressure recry-stallization of pharmaceuticals & other molecular compounds	**Roger Fourme HP** crystallography of biomolecules. Technical aspects	**Vladimir Solozhenko** High-pressure synthesis of novel superhard phases in the B-C-N-O system
10.30	**Coffee**	**Coffee**	**Coffee**	**Coffee**	**Coffee**	**Coffee**	**Coffee**	**Coffee**	**Coffee**
11.00 – 11.45	**Przemek Dera** All different flavors of synchrotron x-ray diffraction at high pressure	**Elena Boldyreva** Anisotropic compression. What can it teach us about intermolecular interactions?	**Alain Polian** Boron and Boron-rich solids at high pressures	**Piero Macchi** Semi-empirical & *ab initio* quantum chemistry description of solid state phases under HP: Chemical applications	**Paul McMillan** HP synthesis of advanced materials	**Nicola Casati** The effect of high pressure on intramolecular geometry	**Paulo Freire** Pressure-induced phase transitions in crystalline amino acids. Raman spectroscopy and X-ray diffraction	**Roger Fourme** HP crystallography of biomolecules. Recent achievements	**Natalia Dubrovinskaia** Structure-properties relationship in novel HP materials
11.45 – 12.30	**Mohamed Mezouar** Synchrotron high-pressure high/low temperature techniques	**Andrzej Katrusiak** Structural studies of phases crystallized at HP as a tool of understanding intermolecular interactions	**Crystelle Sanloup** Amorphous materials at high pressure	**Igor Abrikosov** First principles simulations of alloy thermodynamics in megabar pressure ranges	**Yanbin Wang** Elasticity, plasticity and rheology of materials	**Fernando Rodriguez** Jahn-Teller systems at high pressure	**EXC 2**	**Sebastien Merkel** Experimental study of plastic properties of minerals under pressure	**Bjorn Winkler** Synthesis and structure-property relations of binary metal carbides studied in laser heated diamond anvil cells and with density functional theory calculations
12.30 – 14:00	**Lunch on site**	**Lunch while "watching" Poster Session 1**	**Lunch on site**	**Lunch during EXCURSION 1**	**Lunch while "watching" Poster Session 2**	**Lunch on site**	**Lunch during EXCURSION 2**	**Lunch on site**	**Lunch on site**

14 :00 – 14.45	**Anatoly Balagurov** Present day high-intensity and high-resolution neutron diffraction and neutron scattering at high pressure	**Vladimir Dmitriev** General introduction into the theory of phase transitions	**Paul McMillan** X-ray diffraction of polyamorphic materials and amyloid fibrils at high pressure	**Short boat trip. Extensive walk Mothia Island, Phoenician Archaeology or (free choice) Trapani beach**	**Jens Kreisel** Effect of high-pressure on functional dielectric perovskite-type oxides	**Jennifer Jackson** Phase transitions in the deep Earth: Relationship with seismic observations	**EXC 2 to Selinunte + Segesta, greek archaeology, or (free choice) S Vito lo Capo beach**	**Leonid Dubrovinsky** Effect of spin transitions in iron on structure and properties of Mantle minerals	**Alfonso San Miguel** Raman spectroscopy at high pressure : carbon nanotubes
14 :45 – 15 :30	**Jennifer Jackson** Synchrotron- based spectroscopic techniques: Mossbauer and high-resolution inelastic scattering	**Heidrun Sowa** Phase transitions in AB systems. Symmetry aspects	**15.00:16.30 S Rocco Lecture Hall A round-table discussion (4):** Processing diffraction data collected in the DAC **Leaders / short presenters**: Nicola Casati, Andrzej Katrusiak, Diego Gatta, Przemek Dera, Francesca Fabbiani **Any other contributors are welcome!**	**EXC 1**	**J.-P. Itie** Local aspects of high-pressure transitions in ferroelectrics. X-ray absorption spectroscopy	**Olga Degtyareva** Simple metals at high pressure	**EXC 2**	**John Loveday** Neutron diffraction: Current state of the art and future challenges	**Colin Pulham** High-pressure studies of energetic materials
15.30 – 16.00	**Coffee**	**Coffee**	**16.30: 17.00 Coffee at S Rocco Breakfast room**	**EXC 1**	**Coffee**.	**Coffee**	**EXC 2**	**Coffee**	**Coffee**
16.00 – 16.45	**Leonid Dubrovinsky** Measurements of electrical resistivity at high pressures	**Yaroslav Filinchuk** Light metal hydrides under non-ambient conditions: probing chemistry by diffraction?	**17.00: 17.45 S. Rocco Lecture Hall Short presentations of posters for the two Poster Sessions**	**EXC I**	**Yanbin Wang** Large volume press techniques	**Giovanni Hearne** Nanomaterials at high pressures. Spectroscopy and diffraction techniques	**EXC 2**	**Diego Gatta** Microporous materials at high-pressure: are they really soft?	**John Parise** Analysis of the total scattering using the quantitative HP pair distribution function: I. Practical considerations
17.00 – 18.00	**Introduction into Workshops**	**Follow-Me Workshop 2**: Structure solution from powder diffraction data (S Domenico, 17.00 :18.15)		**EXC I**	**Follow-Me Workshop 5**: Quantum-mechanical calculations on molecular solids (S Domenico, 17.00 :18.15)	**Workshop 7**: Getting the texture information from a 2D dataset; strain analysis **Leader:** to be anounced	**EXC 2**	Lecture on the effect of Mafia in Sicily	**Lars Ehm** Analysis of the total scattering using the quantitative HP pair distribution function: II. Case studies (17.00:17.45)
18.00 – 19.00	**Follow-Me Workshop 1**: DAC handling, HP crystallization (S Domenico)	**Follow-Me Workshop 3**: EOS calculations (S Domenico, 18.15:19.30) **Hands-On Supplement to Workshop 2**: (Madonna room, 18.15:19.30)	**Poster session 1 in San Francesco Court**	**Return to Erice at 19 00**	**Follow-Me Workshop 6**: Ab initio crystal structure prediction (S Francesco, 18.30 :19.45) **Hands-on Supplement to Workshop 3**: (Madonna room, 18.15:19.30)	**Poster Session 2 in San Francesco Court**	**EXC 2**	(start at 17.30) Special lecture: **W. Grochala** The Chemical Imagination at Work in Very Tight Places (MO approach to interpret HP phenomena)	*Closing remarques*
20.00	**Welcome Buffet Dinner+Folk Show (at S. Francesco)**	**Dinner**	**Pasta party (at S. Francesco)**	**Dinner**	**Dinner**	**Pizza party (at S. Francesco)**	**Dinner in front of the Segesta Temple**	**Dinner**	**Good-Bye Buffet Dinner**

Report

The International School of Crystallography, 41st Course:
From Novel Experimental Approaches to Applications in Cutting-Edge Technologies"
4 - 14 June 2009, Erice- Sicily, Italy

Organizers:
E.V. Boldyreva (Novosibirsk State University and the Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the RAS, ul. Kutateladze, 18, Novosibirsk, 630128, Russian Federation; Tel: +7-383-363-4272, Fax: +7-383-363-4132, e-mail: boldyrev@nsu.ru)
P. Dera (CARS, the University of Chicago, ANL, 9700 South Cass Ave., Bldg 434B, Argonne, IL 60439, USA; Tel: +1-630-252-0419; Fax: +1-630-252-0436, e-mail: dera@cars.uchicago.edu

N. Dubrovinskaia served as a coordinator for the theoretical session of the School (Institute of Earth Sciences, Heidelberg University, Im Neuenheimer Feld 236 D-69120 Heidelberg Germany, Tel: +49-6221/54-85 33; Fax: +49-6221/54-48 05; E-mail: Natalia.Dubrovinskaia@min.uni-heidelberg.de)

Summary

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

The School was devoted to the theme of crystallographic studies at high pressure with emphasis on the phenomena characteristic to the compressed state of matter, as well as experimental and theoretical techniques, used to study these phenomena. The agenda of the School naturally encompassed elements of physics (properties and structure), chemistry (chemical reactions, transport), materials science (new materials) and engineering (mechanical properties); in addition it covered 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, des-activation of viruses and toxins). More detailed information can be found on the meeting website http://crystalerice.org.
The Erice Schools had a program of 10 days of intensive training and interaction, and was attended by one hundred twenty two participants (56 lectures were given by 46 speakers). The school had a unique format, truly focused on education, which emphasized direct hands-on exercises and stimulated active interaction between the instructors and the students.

The field of theoretical studies at high pressure is dynamically expanding and the School gave an up-date of the state of affairs in this field for young scientists and students. **‘Theoretical**

methods for high-pressure science' was one of the main topics of the School that reinforced theoretical aspects of the meeting.
S. Scandolo (Italy) gave a review of some fundamental aspects of atomistic simulations in high pressure research, including the construction of the interatomic potentials and the basic methods to sample the constant-pressure and constant-temperature statistical ensemble. I.A. Abrikosov (Sweden) outlined recent developments of theoretical methodology for first-principles simulations of alloys at high pressure. Particular attention was paid to the techniques for a treatment of solution phases. B. Winkler (Germany) spoke about both experimental and theoretical approaches to studies of the role of hydrogen bonding in minerals at high pressure. P. 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.
A Workshop on theoretical calculations of organic, organometallic, coordination compounds at high pressures was given by P. Macchi.

Abstracts of the lectures at the theoretical session.

FIRST-PRINCIPLES SIMULATIONS OF ALLOY THERMODINAMICS IN MEGABAR PRESSURE RANGE

SHORT TITLE: SIMULATIONS OF ALLOY THERMODYNAMICS

IGOR A. ABRIKOSOV

Department of Physics, Chemistry and Biology, Linköping University, Sweden

Abstract. We outline recent developments of theoretical methodology for first-principles simulations of alloys at high pressure. Particular attention will be paid to the techniques for a treatment of solution phases. Limitations of the present-stage theory are discussed, and a necessity to having a close collaboration between theory and experiment are emphasized. We show several examples where the collaboration leads to new discoveries important for physical and geophysical communities.

Keywords: Ab initio simulations; phase stability; alloys; high-pressure

AB INITIO QUANTUM CHEMISTRY AND SEMI- EMPIRICAL DESCRIPTION OF SOLID STATE PHASES UNDER HIGH PRESSURE: CHEMICAL APPLICATIONS

QUANTUM CHEMICAL METHODS

PIERO MACCHI

Laboratory of Chemical Crystallography,
Department of Chemistry and Biochemistry,

University of Bern, Freiestrasse 3, CH-3012 Bern

Abstract. There is nowadays a consensus that the structures of crystals at high pressure provide useful chemical information, at least in three important fields: a) discoveries of new polymorphs and mechanisms of solid-solid transitions or high pressure crystallizations; b) intra- and inter-molecular bonding as a function of the external stress; c) structure-property correlation. While experimental evidence is vital at high pressure, there is an increasing need of support from theoretical predictions, in particular for: a) new phases and structures; b) mechanisms of phase transformations; c) rationalization of the material properties. A brief survey of quantum mechanical descriptions of the solid state is given to summarize the state of the art in the field and the potential developments. Some examples illustrate the successful synergy between theory and experiment.

Keywords: *ab initio* calculations, quantum chemistry, semi-empirical modeling, high pressure

FIRST-PRINCIPLES MOLECULAR DYNAMICS AND APPLICATIONS IN PLANETARY SCIENCE

Sandro Scandolo

The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy
INFM-CNR Democritos National Simulation Center, Trieste, Italy

Abstract. I will review some fundamental aspects of atomistic simulations in high pressure research, including the construction of the interatomic potentials and the basic methods to sample the constant-pressure and constant-temperature statistical ensemble. I will also present a couple of examples where such methods have been used to describe materials of planetary interest.

Keywords: Ab-initio molecular dynamics, interatomic potentials, phase transitions, planetary science

Full lectures are available at:
http://cars9.uchicago.edu/surfacewiki/HPCrystallography/Erice2009/LecturePresentations

Psi-k Network : Towards Atomistic Materials Design

Psi-k
Daresbury Science & Innovation Campus
Daresbury, Warrington
WA4 4AD
UK

Tel: +44 (0)1925 603227
Fax: +44 (0)1925 603634

PSI-K WORKSHOP FINANCE REPORT

Title of the Workshop	**International School of Crystallography, 41st Course**
Workshop Organisers	Prof. E.V. Boldyreva (RU), P. Dera (USA)
Location of the Workshop	Erice- Sicily, Italy
Dates of the Workshop	4 - 14 June 2009
Total Grant from Psi-k	5800 €

EXPENDITURE

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	**Travel**	**Accommodation**	**Total (€'s)**
Prof. I. Abrikosov (SE)	€	€	€
Dr. N. Dubrovinskaia (DE)			
Ms N. Efros (UA)			
Ms I Tyagur (CZ)			
Mr K. Djubek (PL)			
		Total Travel & Accommodation	**€**

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	**Tea / Coffee**	**Lunch / Dinner**	**Total (€'s)**
	€	€	€
		Total Refreshments	**€**

MISCELLANEOUS EXPENDITURE	
Details	**Total (€'s)**
	€
Total Miscellaneous	**€**

Total Travel & Accommodation	**€**
Total Refreshments	**€**
Total Miscellaneous	**€**
TOTAL EXPENDITURE	**€ 5800**