

“Methods of high-pressure single-crystal x-ray diffraction”

A satellite workshop of the 26th European Crystallographic Meeting

Darmstadt (Germany), September 3-4 (2010)

Single-crystal diffraction provides the most accurate structural data on the compression mechanisms of solids. Its methods for high-pressure studies developed over the last three decades are mature and easy to use in both the laboratory and at synchrotron sources. The aim of this workshop is to demonstrate how to perform single-crystal high-pressure X-ray diffraction measurements in diamond anvil cells, to complete the data reduction and analysis, and to obtain the highest-quality data. The workshop will include both lectures and hands-on exercises. It will be suitable for researchers at all levels. Experience in single-crystal X-ray diffraction will be assumed, but no previous experience in high-pressure methods is necessary. Participants who have already collected high-pressure data are encouraged to bring their own problematic datasets for discussion and analysis. Different data processing strategies and programs will be presented. The workshop will be interactive through informal discussions and small round tables of specific interest groups, e.g., the software fayre.

Registration: <http://conventus.de/index.php?id=registration>

Topics and schedule

Morning session (September 3rd, 2010; 8:30-12:00)

Introduction to high-pressure single-crystal x-ray diffraction (Ross Angel)

Time: 45 minutes

Designing the experiments (Ronald Miletich, Benedetta Periotto)

Types of diamond anvil cells (ETH, Almax, Ahsbahs, Merrill-Bassett, etc.)

Preparing single crystals and loading diamond anvil cells

Pressure transmitting media and pressure calibration

Laboratory and synchrotron facilities

The choice of CCD, image plate, and point detectors for different crystallographic problems:

molecular systems, inorganic materials, modulated structures, superstructures, diffuse

scattering, twinning, polytypes

Time: 2 hours

Data collection strategies using area and point detectors (Clivia Hejny)

Crystal orientation and centering

Optimization of data collection parameters

Data coverage, redundancy

Time: 45 minutes

Afternoon session (September 3rd, 2010; 13.30 – ∞)

Software fayre: going from raw data to hkl file (Matteo Alvaro)

Area detectors:

Oxford Diffraction (Diego Gatta, Fabrizio Nestola)

Bruker (Tonci Balic-Zunic)

STOE (Andrzej Grzechnik, Karen Friese)

XDS (Andrzej Grzechnik, Karen Friese)

Point detectors:

WinIntegrStp (Ross Angel)

Time: depends on the participants

Morning session (September 4th, 2010; 8:30 – 12:00)

Equations of state (Tiziana Boffa-Ballaran)

Time: 2 hours

Data reduction and analysis (Karen Friese, Ross Angel)

Systematic errors and data quality

Absorption corrections, averaging

Structure refinement methods and tricks

Time: 1.5 hours

Afternoon session (September 4th, 2010; 13:30 – 18:30)

Structure validation (Tonci Balic-Zunic, Karen Friese)

cif, crystal chemistry

Time: 1 hour

Open session: more tutorials, exercises & discussions (all speakers)

Time: 4.5 hours

Speakers

Matteo Alvaro (Virginia Polytechnic Institute and State University, USA)

Ross Angel (Virginia Polytechnic Institute and State University, USA)

Tonci Balic-Zunic (University of Copenhagen, Denmark)

Tiziana Boffa-Ballaran (University of Bayreuth, Germany)

Karen Friese (University of the Basque Country, Spain)

Diego Gatta (University of Milan, Italy)

Andrzej Grzechnik (University of the Basque Country, Spain)

Clivia Hejny (University of Innsbruck, Austria)

Ronald Miletich (University of Heidelberg, Germany)

Fabrizio Nestola (University of Padova, Italy)

Benedetta Periotto (University of Copenhagen, Denmark)