The 2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School
University of Edinburgh, Scotland, 2024

Brief Background

The 2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School will take place at the University of Edinburgh (Edinburgh, Scotland) from Monday July 22nd to Friday July 26th 2024 inclusive. This five-day long School aims at providing an introduction to a novel method of single-crystal X-ray diffraction (SCXRD) structure studies at extreme pressures generated in a diamond anvil cell to early career stage scientists (master and PhD students, post-docs) and established scientists working in the field of high pressure research. The recent methodological advancements in high-pressure SCXRD drastically extends its applications, previously mostly limited to ~20 GPa and large single crystals, now reaching hundreds of GPa and temperatures of thousands of degrees on submicron-sized polycrystalline aggregates. An overview of the necessary fundamental theoretical and methodological principals, including diamond anvil cell preparation, strategy of experiments, laser-heating, introduction to software and SCXRD, will be covered through lectures accompanied by demonstrations, hands-on sessions, and step-by-step tutorials. At the end of the School, participants are expected to be able to perform basic high-pressure SCXRD experiments, as well as data processing and interpretation.

The School is building on the huge success of the previous Summer School held in Bayreuth, Germany, in 2020 (https://www.dubrovinskaia.uni-bayreuth.de/en/High-Pressure-Summer-School-2020/index.html).

Details of the School

The School will be held in the James Clerk Maxwell Building of the University of Edinburgh's King's Buildings campus. The James Clerk Maxwell Building is well equipped to host the School, housing modern lecture halls and computer laboratories; the latter essential for the planned hands-on sessions and step-by-step tutorials. The university also provides reasonably-priced catering services that can accommodate various dietary preferences and can serve snacks and coffee on breaks, as well as lunch and dinner. The School aims at welcoming at maximum of 30 participants from across the globe.

Members of Committee and Organisers

Dr Dominique Laniel (University of Edinburgh, United Kingdom; local organizer)
Prof Dr Dr hc Natalia Dubrovinskaia (University of Bayreuth, Germany)
Prof Dr Dr hc Leonid Dubrovinsky (University of Bayreuth, Germany)
Prof Dr Elena Bykova (Goethe University Frankfurt, Germany)
Prof Dr Maxim Bykov (Goethe University Frankfurt, Germany)

Summer School Plan

The recent developments in high-pressure single-crystal X-ray diffraction are game-changers for our field of research. As developers and experts of this method, we feel that it is essential for the community to learn about this approach, hence the organisation of the School. The School will be roughly divided into five learning modules: i) *Experimental basics of high pressure*; ii) *Fundamentals of crystallography and single-crystal X-ray diffraction*; iii) *Tools, methods and software for single-crystal X-ray diffraction*; iv) *Examples and applications*; and v) *Hands-on workshops*. Due to the emphasis on the attendees being able to use this technique by the end of the summer school, about 40% of the time will be spent on the hands-on workshop.

i) The *Experimental basics high-pressure* module covers an introduction to diamond anvil cells (DACs) and their preparation, pressure determination, and equations of state. It includes methods of heating and cooling in DACs, such as resistive and laser heating, and cryogenic cooling. The module also introduces synchrotron X-ray sources, focusing on the capabilities of synchrotron facilities for single-crystal X-ray diffraction in DACs.

ii) The *Fundamentals of crystallography and single-crystal X-ray diffraction* module covers essential topics in crystallography and diffraction. Attendees will be introduced to crystal symmetry, including symmetry operations, space groups, and reflection conditions. The module will also explain X-ray diffraction principles, Bragg's Law, and the advantages of single-crystal X-ray diffraction. Attendees will gain insights into challenges and approaches to solving crystal structures, including the phase problem and Fourier transformation. Additionally, the lectures will provide a short historical overview of high-pressure crystallography and its development, highlighting double-stage DACs and ultra-high pressure studies.

iii) The *Tools, methods, and software for single-crystal X-ray diffraction* module covers essential topics in data processing, software utilization, and crystallographic analysis. Attendees will be introduced to the CrysAlis^{Pro} software package, including data conversion, peak search, indexing, and intensity extraction. The module also explores crystal structure visualization using the VESTA software. Participants will gain insights into OLEX2, a software package for single crystal data treatment and refinement. The module also addresses common issues in high-pressure datasets and helpful tools for data validation. Techniques for identifying twinned crystals, refining

twinned data, and understanding warning signs of twinning will be covered. Disorder and modulation, and how to account for them, will also be part of the learning material.

iv) The *Science* lectures will provide the attendees with scientific cases highlighting the power of the novel methodology for high-pressure single-crystal X-ray diffraction. These lectures will cover different subfields of high-pressure research, namely physics, chemistry and geology.

v) The *Hands-on workshops* will give the attendees the opportunity to themselves test the knowledge learned during the lectures and gain a practical understanding of the various concepts and software. This includes data analysis in the Crysalis^{Pro} software, structure determination and refinement in the OLEX2 software and structure visualisation using VESTA. The participants will be divided into small subgroup of about five individuals, and training datasets of increasing difficulty will be provided to them along with step-by-step instructions. Instructors will circulate the rooms to help out with any difficulties. The instructors will be some of the organizers as well as PhD and post-doctoral students at the University of Edinburgh.