2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School

Organizers: Dominique Laniel, Elena Bykova, Maxim Bykov, Leonid Dubrovinsky, Natalia Dubrovinskaia

The 2nd High-Pressure Single-Crystal X-Ray Diffraction Summer School was held at the James Clerk Maxwell Building of the University of Edinburgh (Edinburgh, Scotland), from July 22nd to July 26th 2024 (https://indico.ph.ed.ac.uk/event/282/overview). The School was generously supported and approved by the Scottish Universities Summer School in Physics. A total of 30 participants from fifteen countries and four continents attended the full week. Out of these, seven were from institutions in the United Kingdom, (four from Scottish Universities and three from English Universities), while all others were international. Participants were provided an accommodation at the University's Pollock Halls. The School was such a vibrant success that we will hold another one next summer, but this time in Frankfurt (Germany)—and certainly upcoming years as well, making it an annual event.

Group picture taken during the School, with participants and lecturers present. The picture was taken in front of the Centre for Science at Extreme Conditions (CSEC) of the University of Edinburgh.

The intent of the School was to train young and established scientists in the recent methodological advancements in high-pressure single-crystal X-ray diffraction. These new developments enable solving and refining crystal structures from tiny micron- to submicron-sized crystallites confined in diamond anvil cells up to pressures of multiple hundreds of gigapascals (GPa). 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, were covered through lectures. These were accompanied by thirteen hours of hands-on sessions, where participants were divided into five small groups of six individuals, each with its own instructor, and guided through step-by-step tutorials and examples (see School's schedule below). At the end of the School, participants were able to perform basic high pressure SCXRD experiments, as well as data processing and interpretation. The lectures and hands-on tutorials were given by a total of ten experts, including three from the United Kingdom (Dominique Laniel, Miriam Pena-Alvarez, Simon Parsons), five from Germany (Natalia Dubrovinskaia, Leonid Dubrovinsky, Maxim Bykov, Elena Bykova, Konstantin Glazyrin) and one from the United States (Stella Chariton), with a woman-to-man ratio of 4:6.

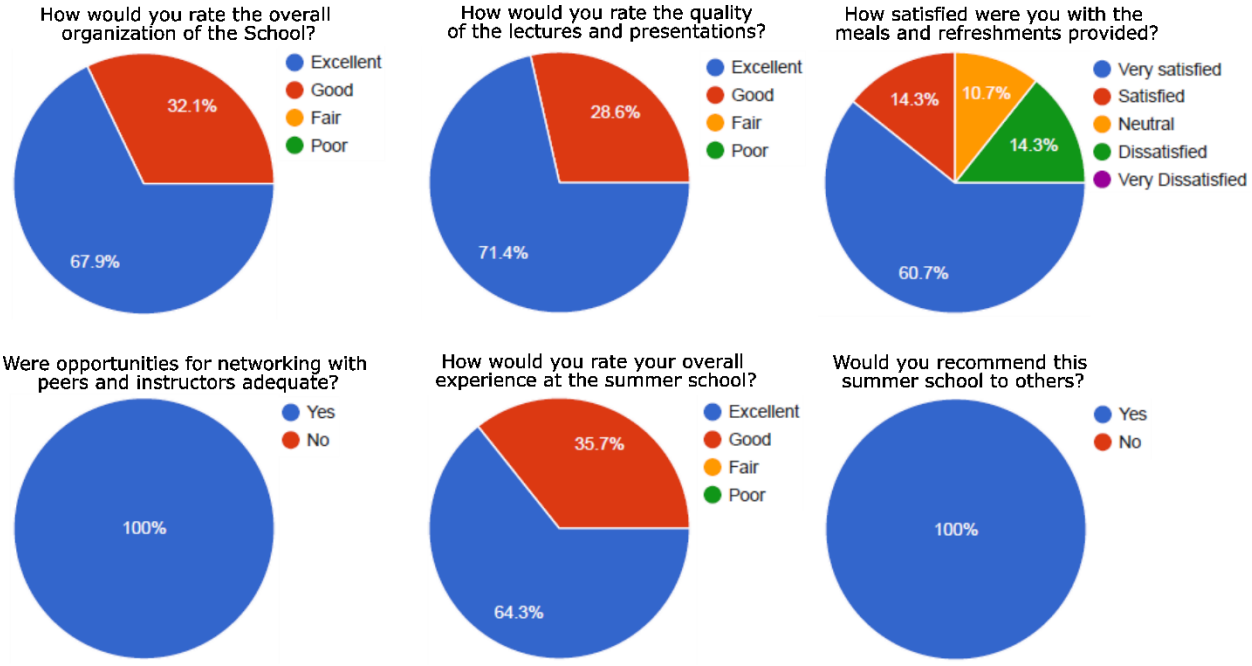
Time	Monday, July 22nd	Tuesday, July 23rd	Wednesday, July 24th	Thursday, July 25th	Friday, July 26th
8:30-9:00	Onsite Registration				
9:00-10:00	Opening Remarks Historical overview and perspectives of HP crystallography (**ND**)	Basics of DACs Pressure determination Equation of state (**MPA**)	Acquiring good SCXRD data in DACs (**DL**)	Processing HP data: problems and helpful tools for their solution (**SP**)	Dealing with complex datasets. Part III. (disorder) (**EB**)
10:00-10:15	Break	Break	Break	Break	Break
10.15-11.15	Periodicity, lattices and symmetry (**LSD**)	Heating and cooling in DACs (**KG and BM**)	Crystal structure visualization and HP crystal chemistry (**MPA**)	Dealing with complex datasets. Part I. (twinning) (**EB**)	Getting the most out of your SC data (**LSD**)
11.15-12:00	CSEC Laboratory tours (LVP, LH, Raman)	Solving crystal structures. Part II. (Structure analysis: the phase problem, refinement) (**DL**)	CSEC Laboratory tours (LVP, LH, Raman)	SC data validation (**EB**)	CSEC Laboratory tours (LVP, LH, Raman)
12:00-13:00	**LUNCH**	**LUNCH**	**LUNCH**	**LUNCH**	**LUNCH**
13:00-14:00	Solving crystal structures. Part I. (Diffraction, Bragg's law, structure factors and Fourier transforms) (**MB**)	APS facility: the 13IDD beamline **(SC)**	Introduction to Shelx and OLEX2 (**EB**)	Dealing with complex datasets. Part II. (modulation) (**MB**)	Hands-on: Mapping and analysis of complex samples *6 groups*
14:00-15:00	Introduction to the CrysalisPro software + DAFi (**LSD**)	Hands-on: Simple cases with CrysalisPro *6 groups*	Hands-on: More complex cases with CrysalisPro *6 groups*	Hands-on: Structure solution and refinement *6 groups*	Hands-on: Mapping and analysis of complex samples *6 groups*
15:00-15:15	Break	Break	Break	Break	**Concluding Remarks**
15:15-17:00	Hands-on: Getting started with CrysalisPro (calibration + beginning simple case) *6 groups*	Hands-on: More complex cases with CrysalisPro *6 groups*	Hands-on: Structure solution and refinement *6 groups*	Hands-on: Structure solution and refinement *6 groups*	
17:00-18:00	**Whiskey tasting**	Posters	**Science talk**	Posters	
18:00-20:00	**DINNER**	**DINNER**	**DINNER**	**DINNER**	

* for all hands-on sessions, there will be 6 instructors (post-docs, PhDs and some lecturers)

EB = Elena Bykova; ND = Natalia Dubrovinskaia; MPA = Miriam Pena-Alvarez; SC = Stella Chariton; SP = Simon Parsons; KG = Konstantin Glazyrin; BM = Bernhard Massani; LSD = Leonid Dubrovinsky; MB = Maxim Bykov; DL = Dominique Laniel

To maximize discussions between participants as well as between participants and lecturers, snacks, lunches and dinners were provided onsite for the complete duration of the School. All participants were requested to bring a poster presenting their research, which were shown and displayed during two poster sessions. Moreover, extracurricular activities took place during three evenings, namely a whisky tasting, a walking tour of Edinburgh and a ceilidh—a traditional Scottish group dancing.

During the last day of the School, the participants were requested to fill out an online survey to gauge their satisfaction and identify aspects to improve for next editions of the School. Overall, their response was overwhelming positive. Indeed, all 28 participants that took part in the survey said they would recommend the School to others, while 64.3% and 35.7% rated their overall impression of the School as "Excellent" or "Good", respectively. Among all surveyed aspects, the one with the least positive feedback was meals and refreshments, for which 75% of the participants were either "Very satisfied" or "Satisfied", but 25% were "Neutral" or "Dissatisfied". In the future, a different catering company will be used.



Questions and pie chart representations of the answers obtained from the survey filled out by 28 participants at the end of the School.

The School's total expenditure was of £22,629 while the total income was of £24,037. The income came from various funding sources including SUSSP, the International Union of Crystallography (IUCr), Rigaku, the Cambridge Crystallography Database Centre (CCDC)—with the largest contribution coming from SUSSP. Through this funding, the cost of the students' registration fees was decreased by half, and the transport fees of two European speakers fully covered. The surplus of £1,408 will be returned to SUSSP.

Given the increasing importance diamond anvil cell single-crystal X-ray diffraction of polycrystalline samples methodology, as well as the very positive feedback received from participants, we

are confident that new participants will attend the next edition in Frankfurt (Germany), which will undoubtedly be just as successful. Looking forward to summer 2025…!