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Editorial

Status of third-generation synchrotron crystallography beamlines: An overview

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Crystallography, the branch of science devoted to the study of molecular and crystalline structure and properties, with far-reaching applications in mineralogy, chemistry, physics, mathematics, biology and materials science, as defined in *A little dictionary of Crystallography* (International Union of Crystallography, 2014), and synchrotron beamlines are the object of this *Focus Point*. Undoubtedly this is an extremely successful combination, synchrotron beamlines being one of the main tools to tackle crystallography problems. On the other hand, crystallography-based experiments account for a very relevant fraction of the science done nowadays in synchrotrons. The number of facilities and beamlines therein has grown rapidly during the last years. This issue aims at providing a summary of the situation.

Initially motivated by the celebration of the international year of Crystallography in 2014, this endeavor has continued during 2015 and 2016 in order to complete a coherent collection of papers summarizing the status of third-generation synchrotron beamlines devoted to crystallography. Europe was chosen as the target scope for the issue and most facilities have finally agreed to contribute with a paper, thereby providing a practically exhaustive *map* of crystallography-devoted beamlines. For the sake of illustrating the parallel efforts being done elsewhere, an invited contribution by the Shanghai Synchrotron Radiation Facility, serving the rapidly evolving Chinese scientific community, was also taken on board.

The issue includes 9 papers for 9 facilities. For the convenience of the reader the structure of the papers has been standardized to some extent. Each of them starts with a brief facility introduction, gives an overview of crystallography beamlines therein, describes in detail one or a few selected ones and presents examples of relevant scientific highlights. Emphasis has been made, wherever possible, on technical details and design choices (with many pictures and schematics), in such a way that the reader can compare and get a comprehensive view of the different instrumentation approaches used by each facility. Additional information is also offered on future plans and complementary support facilities.

The paper by Lausi *et al.* (Eur. Phys. J. Plus **130**, 43 (2015)) presents crystallography beamlines at Elettra. This facility operates both a storage ring working at 2.0 and 2.4 GeV and a free electron laser (FERMI). The storage ring hosts 26 beamlines, out of which 4 are dedicated to crystallography. These four beamlines are briefly addressed, with their key parameters summarized in a very useful table. Then one of the beamlines, XRD2, dedicated to macromolecular crystallography, is covered in further detail. XRD2 is a new tool, set up recently by Elettra, to cope with *the exponential growth of structural biology*, citing literally the paper. Very interesting scientific highlights are presented covering different areas of knowledge, from oxygen order in a cuprate superconductor to growth of semiconductor nanowires or Alzheimer's disease.

Logan *et al.* (Eur. Phys. J. Plus **130**, 49 (2015)) account for the status at the Max IV facility, where a new world-leading emittance storage ring has come into operation during 2016. There are three beamlines, with four end stations devoted to crystallography currently in operation in the Max II 1.5 GeV storage ring. One of the beamlines, I911, is described with particular level of detail. On the other hand, the new ultra-low-emittance ring will host a total of five beamlines devoted to crystallography experiments, briefly addressed in the paper: a beam size of $1 \times 1\,\mu\text{m}^2$ with high flux on sample is targeted for the future macromolecular crystallography beamline MicroMAX, which will then become a cutting edge tool. Scientific highlights are identified and briefly explained, with additional information available in the references, from Huntington's or Alzheimer's diseases to hydrogen fuel cell or lithium battery research.

Crystallography beamlines at the Diamond Light Source are covered in the paper by Allan *et al.* (Eur. Phys. J. Plus **130**, 56 (2015)). The instrument portfolio presented in this case includes eight beamlines for macromolecular crystallography, two of them in design stage at the moment of writing the paper, plus four beamlines devoted to crystallography in the field of Physical Sciences. Several of these beamlines are described with remarkable level of detail, including the four ones working in the area of Physical Sciences and two Life Science ones. One very interesting case is that of the long-wavelength macromolecular crystallography beamline, wherein a rather unique in-vacuum detector system is used to measure small anomalous signals from sulphur and phosphorous. A specific section is available on support laboratories. Scientific highlights are in this case organized on a per-beamline basis, within the same section devoted to beamline description. Some examples are: studies of magnetic domains in perovskites, highly exotic clusters like a Cd66 core with an organic shell of ligands or structural studies of the foot-and-mouth disease virus (FMDV).

Mueller-Dieckmann *et al.* (Eur. Phys. J. Plus **130**, 70 (2015)) present the status at the European Synchrotron Radiation Facility (ESRF), concentrating in this case only on macromolecular crystallography (MX) beamlines. As the first European third-generation facility the ESRF has long been contributing to MX, which makes particularly useful the historical perspective adopted in the introduction section. In total the ESRF hosts eight stations devoted to MX or Bio-SAXS, two of them corresponding to collaborative research group (CRG) beamlines. After a comprehensive overview the focus is placed on the expected performances after the ambitious machine upgrade planned for the near future, which will massively improve the flux on sample and allow to move into micron-sized beam spots. The set of end stations served from the ID30 straight section, as the newest tools at the ESRF for MX are then described in detail. Scientific highlights are mainly given in the shape of references to well-known cases, such as the contributions to the structural determination of the ribosome (B.T. Wimberly *et al.*, Nature **407**, 327 (2000) and J. Harms *et al.*, Cell **107**, 679 (2001)) and of G-coupled protein receptors (S.G.F. Rasmussen *et al.*, Nature **450**, 383 (2007) and T. Warne *et al.*, Nature **454**, 486 (2008)), both leading to Nobel Prize for Chemistry in 2009 and 2012, respectively.

Bessy II beamlines are the scope of the paper by Mueller *et al.* (Eur. Phys. J. Plus **130**, 141 (2015)). As in the case of the ESRF, BESSY II has chosen to concentrate exclusively on its MX portfolio, which includes three beamlines. All of them are described with a very comprehensive table, pictures and schematics. Particular attention is paid to complementary utilities, such as support labs and computational tools. Finally scientific highlights are given, including in-house research efforts on fragment screening and long wavelengths for structure determination, and external user results such as new cancer target proteins or enzymes useful for clean production of hydrogen.

The young facility ALBA is covered in the paper by Fauth *et al.* (Eur. Phys. J. Plus **130**, 160 (2015)). ALBA, based on a 3 GeV storage ring, started operation with users in 2012. Two beamlines are devoted to crystallography experiments and both are presented in a particularly high level of detail in this paper: BL13-XALOC targeted at MX and BL04-MSPD dedicated to powder diffraction, the latter having two end stations. Some scientific highlights are given, such as studies on Auxin Response Factors, determination of the crystal structure of novel zeolites or *in operando* studies of electrochemistry processes in materials for batteries.

The paper by Burkhardt *et al.* (Eur. Phys. J. Plus **131**, 56 (2016)) addresses macromolecular crystallography beamlines at PETRA III. Three beamlines are addressed, one of them operated by DESY and the other two by EMBL. Beamline P11 is chosen for a detailed description. The very low emittance provided by the PETRA III ring allows to serve this interesting tool with enough photon flux on a spot size as small as $1 \times 1\,\mu\text{m}^2$. A particularly detailed explanation of the corresponding instrumental challenges is given: optics layout, feedback systems, etc. It is therefore not surprising that serial crystallography is one of the fields chosen to report on scientific highlights (F. Stellato *et al.*, IUCrJ **1**, 204 (2014)). Very useful information is given on essential complementary tools, such as sample preparation and computational infrastructure.

Crystallography beamlines at Soleil are the topic of the paper by Coati *et al.* (Eur. Phys. J. Plus **132**, x (2017)). Eight beamlines are addressed, with all key parameters described in a comprehensive table. PROXIMA1, devoted to macromolecular crystallography, is described in a dedicated section. Remarkable level of detail is given in all key elements therein, nicely complemented with pictures and technical references, in such a way that all key technical choices are not only described, but conveniently justified by scientific case-driven performances. Scientific highlights are focused on phasing experiments using weak anomalous signals, again with a remarkably high level of technical detail both on the experimental approach and data analysis, which can be particularly useful to specialized readers.

The Shanghai Synchrotron Radiation Facility operates since 2009, based on a 3.5 GeV storage ring, and is the object of the paper by He and Gao (Eur. Phys. J. Plus **130**, 32 (2015)). This facility has been invited to participate in the present issue, in order to present a very interesting example of development in crystallography beamlines taking place outside Europe. Indeed SSRF and the Chinese scientific community have experienced an impressive growth during the last few years. SSRF operates two beamlines devoted to crystallography: BL17U1 dedicated to macromolecular crystallography and BL14B1 dedicated to physical sciences. The former, wherein impressive productivity figures are reported within its first five years of operation, is described in detail in the paper. Six additional beamlines will be available for crystallography experiments in the ambitious phase two of the facility. Scientific highlights include the structural determination of proteins related to avian flu or promising studies in the field of hydrogen storage, as two selected examples.

Within the nine papers of the issue the reader may find references to more than 50 beamlines available or planned in the close future for crystallography experiments, nicely summarized in a reference table for most of the papers. Detailed technical descriptions of 17 beamlines are given, with additional information about complementary aspects like user access, laboratory support or computational tools. A nice global summary of scientific highlights can be obtained by combining the proper sections of all the papers, very briefly addressed in some cases, but complemented with adequate references. Last but not least, looking through the papers one may get key hints on the future directions as planned by the different facilities. Altogether, an interesting and useful collection to have a global view of crystallography tools and advances in a very significant subset of the worldwide synchrotron network.

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Guest Editors