A Multipurpose X-ray Beamline at ELETTRA: The Scientific Case

The *BOSS* Collaboration

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Abstract:
The scientific case and the conceptual design for the X-ray beamline BOSS (Beamline Of Slovenian Scientists), proposed to be constructed at a bending magnet port of ELETTRA, are presented. The beamline is of the multipurpose type in order to cover at least 70% of the current needs of Slovenian basic, applied and industrial research. The experiments on the beamline will be in the domain of X-ray absorption, fluorescence and electron spectroscopy, and to a certain extent also X-ray scattering.

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1. Introduction

Synchrotron radiation became available in a routine manner to the scientific community in the early 1980s. Since that time the use of techniques employing synchrotron radiation has proliferated, so that the unique properties of this form of electromagnetic radiation are now having a major impact on many areas of natural and technical sciences such as chemistry, material science, physics, biology, biochemistry, pharmacology, ecology, medicine, etc. Not only have new opportunities with existing methodologies been opened up but also several new techniques have become available [1-4].

Another aspect of synchrotron light sources is that they are research centres of national and international excellence. A large number of research fields are being pursued in such centres and many scientific articles and theses are being written. In such places, experts of many different fields meet resulting in cross-fertilisation of ideas and projects.

All the mentioned advantages of synchrotron centres are even further pronounced for Slovenia by the vicinity of ELETTRA. The Trieste synchrotron light source ELETTRA is the world's brightest light source in the UV and soft X-ray region [5]. As such it further extends the possibilities of research with respect to existing light sources. Researchers in Slovenia have therefore established the collaboration BOSS (Beamline Of Slovenian Scientists) which seeks ways to perform research at ELETTRA and to construct the beamline BOSS.

Only the construction of a beamline and its subsequent utilisation will allow Slovenian research groups at universities, institutes and from the industry to fully exploit all possibilities offered by the Trieste light source. By building and operating a beamline, Slovenian researchers will be able to conduct specific types of experiments, suited to their particular needs. In addition, they will be able to access other beamlines by trading beam time.

The proximity of Trieste and Ljubljana will allow also for significant savings in travel costs and laboratory equipment: samples can be brought from the home laboratory to ELETTRA within one hour. Even experiments, for which other quite distant light sources may be slightly better suited, will be therefore performed more efficiently and faster at ELETTRA.

2. Design Considerations

Since the beamline BOSS is a national project, it has to allow as many experiments as possible to researchers from Slovenia, as long as they can be reasonably well performed on BOSS, even though some fields may be covered by other beamlines. Hence BOSS is a multi-purpose beamline, employing the following experimental methods: XAS (X-ray absorption spectroscopy, i.e. XANES - X-ray absorption near edge structure and EXAFS - extended X-ray absorption structure), XRF (X-ray fluorescence) and XPS (X-ray photoelectron spectroscopy), with the possible extension to WAXS (wide angle X-ray scattering), SAXS (small angle X-ray scattering) and XSW (X-ray standing wave).

A recent survey among Slovenian research groups has shown that there is interest practically in all experimental methods that can be offered by ELETTRA. However, more than 70% of the requests can be fulfilled by a single beamline operating in the X-ray region.

The diversity is also reflected in the proposals for experiments on the beamline BOSS, presented in the following section. The proposed research projects can be roughly divided into four groups:

¥ structure determination with EXAFS (proposals 1-17);

¥ atomic physics research with absorption, fluorescence and electron spectroscopy (pr. 18 - 22);

¥ x-ray fluorescence analysis (pr. 23 - 24);

¥ structure determination with x-ray diffraction and small angle scattering (SAXS) (pr. 25 - 29).

One of the main characteristics of almost all of the proposed projects is the combined use of different experimental methods in order to achieve the research goal. The combination of absorption and fluorescence spectroscopy is required in particular for the research in atomic physics (pr. 18, 19, 20), while the combination of x-ray diffraction and absorption or fluorescence spectroscopy for the EXAFS is demanded for structure determination (pr. 8, 10, 12, 13, 14, 16, 17, 25, 26).

About two thirds of the users intend to use absorption spectrometry as the main experimental method (mainly for EXAFS and XANES spectroscopy [6]) (pr. 1 - 10, 12 - 14, 16 - 19, 25). The EXAFS spectroscopy is a particularly interesting method for the industry, too. An analysis of recent industrial use of the SRS at Daresbury [7] shows that 47% percent of the use is allocated to experiments with EXAFS making it the most widely used method for industrial synchrotron radiation research.

The beamline BOSS has been therefore designed primarily for absorption spectroscopy, exploiting the high spectral flux and small source point of the ELETTRA bending magnet. The spectral region covers either the K-edge or the L-edge of almost all elements between and including phosphorous (Z=15) and platinum (Z=78), giving sufficient tunability for a wide range of absorption experiments. The limits actually come from the absorption in the C and Be filters below 2 keV and from the low spectral flux from the source and the poor reflectivity of the gold coated mirror above 12 keV [8].

The expected characteristics of the beamline are [8]:

¥ adjustable photon energy in the range between 2 keV (6.2) and 12 keV (1.0);

¥ Energy resolution of about 3000 or better with more than 10^{12} monochromatized photons/second over the whole spectral region;

¥ small focal spot size on the sample (below 1 mm^2);

¥ vertical divergence below 0.4 mrad.

Fluorescence spectroscopy, which is requested in about half of the proposals (pr. 1, 4, 7, 9, 10, 13, 14, 16 - 25), and photoelectron spectroscopy, requested in 25% of the proposals (pr, 4, 8, 11, 12, 15, 22) covering mainly surface EXAFS and atomic physics research, are also well suited to the characteristics of the BOSS beamline. None of them is covered by other beamlines in the complete range between 2 and 12 keV, although there is a partial overlap with the ALOISA [9] and the EXACT beamline [10]. Both methods can be used as stand-alone research tools, although they will prove even more useful when used in combination with absorption spectroscopy.

X-ray diffraction is requested in 30% (pr. 5, 8, 12, 13, 14, 16, 17, 22, 26, 27, 29) and small angle scattering in 15% of the proposals (pr. 10, 13, 26, 27, 28). X-ray scattering already sees two dedicated beamlines at ELETTRA, the diffraction [11] and the SAXS [12] beamline. However, the characteristics of BOSS allow also a range of scattering experiments and this can be exploited in order to allow Slovenian users immediate usage without having to wait for beam time at the dedicated lines. This is in particular important for the experiments where the samples are analysed with diffraction and absorption or fluorescence spectroscopy at the same time. In addition, BOSS is a possible candidate for anomalous SAXS experiments, which can not be performed on the SAXS beamline, since it operates at fixed wavelengths [12].

The characteristics of BOSS are sufficient also for normal incidence XSW experiments [13], therefore XSW is considered as a potential method even though no proposals were submitted from Slovenian researchers yet. The experiments are quite simple involving only a scan in energy of the incoming radiation instead of a scan in angle.

Since SEXAFS and XSW can use the same beamline and the same experimental apparatus, this is a natural combination of methods for determining surface adsorbate geometries.

The main experimental chamber will be equipped to allow several types of measurements of the absorption coefficient, via the detection of the transmitted flux as well as the secondary processes like fluorescence, photoelectrons and Auger electrons. The chamber will allow the addition of particular sample cells which will allow the study of crystalline, amorphous, liquid and gaseous samples under different temperatures, pressures and other physical and chemical conditions. Measurements of trace elements with XRF will be possible with the same chamber.

Surface science (pr. 4, 11, 15) and some atomic physics experiments (pr. 21, 22) will need dedicated experimental chambers. The Slovenian beam line will deliver the proper type and quality of radiation for these experiments. Attachment ports for several kinds of experimental chambers and detectors are foreseen.

The chambers and specialised detectors will be constructed or are already under construction by individual users: an energy and a wavelength dispersive X-ray spectrometer (pr. 20, 21), an electron energy spectrometer (pr. 22), and a module for total reflection x-ray fluorescence (pr. 23). For high energy resolution experiments an additional four crystal monochromator can be inserted in the beam in front of the experimental chamber to provide very high energy resolution of the incident beam (·E/E about 10000).

For surface mapping, the addition of a glass capillary microprobe is envisaged (pr. 23, 24) giving spatial resolution to all of the aforementioned methods of about 10 - 30 m [14] or even down to 1 m [15]. For higher spatial resolution a PEEM (photoelectron emission microscope) camera could be used, giving a resolution of 0.5 m [16].

3. The List of Proposals for Experiments at BOSS

3.1. Structure Determination with EXAFS

1. *Investigation of the Oxides Films Formed by Oxidation of CrN Hard Coatings by XANES and EXAFS*, I. Milosev et al., Jozef Stefan Institute, Ljubljana
2. *Short Range Determination of Alkoxide Derived Precursors for Functional Ceramics*, M. Kosec et al., Jozef Stefan Institute, Ljubljana
3. *Characterisation of the Sol-Gel Process with X-ray Absorption Spectroscopy,* S. Pejovnik et al., National Institute of Chemistry, Ljubljana
4. *Investigation of the Polymer Electrolyte Structural Determination by EXAFS*, M. Kovac et al., National Institute of Chemistry, Ljubljana
5. *Structural Studies of Non- and Poor Crystalline Coordination Compounds,* P. Bukovec et al., Department of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana
6. *Analysis of $RE_2TM_{17}N_{3-x}$ Compounds by Different analytical Methods,* S. Kobe Besenicar et al., Jozef Stefan Institute, Ljubljana
7. *Determination of Coordination Sphere of Metals in Metal Complexes with Fulvic Acids*, M. Kranjc et al., Jozef Stefan Institute, Ljubljana
8. *Research on Characterisation and Structure of Zeolites and Aluminophosphate Molecular Sieves*, V. Kaucic, National Institute of Chemistry, Ljubljana
9. *Studies of Metal-Containing Liquid-Crystal Systems - Copper Carboxylates and their Derivatives*, P. Segedin et al., Department of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana
10. *Low-angle X-ray Scattering and EXAFS Studies of Sol-Gel Processed Materials*, B. Orel, National Institute of Chemistry, Ljubljana
11. *Study of the Activation Process of Catalytic Probes*, M. Mozetic et al., Institute for Electronics and Vacuum Technology, Ljubljana
12. *Study of Low-Dimensional and Surface Structures,* A. Prodan et al., Jozef Stefan Institute, Ljubljana
13. *Ion Paths in Ion Conducting Polymers*, D. Abramic, Jozef Stefan Institute, Ljubljana
14. *Structural Investigations of Binary Fluorides and Fluorometalate Complexes,* S. Milicev, Jozef Stefan Institute, Ljubljana
15. *XPS and EXAFS Characterization of Surface and Thin Films*, A. Zalar et al., Institute for Electronics and Vacuum Technology, Ljubljana
16. *Organization of Thin Layers of Phospholipids and Other Amphiphiles. Effects of Inclusion and Supporting Materials.*, J. Grdadolnik, National Institute of Chemistry, Ljubljana

17. *Research in Synthesis and Rare Structure Properties of Dimolybdenium(II) Units*, B. Udovic et al., Department of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana

3.2. Atomic Physics Research with Absorption, Fluorescence and Electron Spectroscopy

18. *Multiple Photoexcitation by X-ray Absorption and Fluorescence Spectrometry*, A. Kodre et al., Jozef Stefan Institute, Ljubljana
19. *Study of Relativistic Effects (Breit Interaction) in Atoms by X-ray Absorption and Fluorescence Spectrometry,* A. Kodre et al., Jozef Stefan Institute, Ljubljana
20. *The Study of the De-excitation of Photoelectrically Produced Inner Shell Vacancies*, M. Hribar et al., Jozef Stefan Institute, Ljubljana
21. *Correlated Electron-Photon Decays Following Atomic Inner-Shell Ionisation*, M. Budnar et al., Jozef Stefan Institute, Ljubljana
22. *Correlated Processes in Atoms Studied by Electron Spectroscopy,* Z. Smit et al., Jozef Stefan Institute, Ljubljana

3.3. X-ray Fluorescence Analysis

23. *Synchrotron Radiation X-ray Fluorescence Analysis,* P. Kump, Jozef Stefan Institute, Ljubljana
24. *Life Science Research Using Synchrotron Radiation - Induced X-ray emission (SRIXE),* B. Smodis et al., Jozef Stefan Institute, Ljubljana

3.4. Structure Determination with X-Ray Diffraction and Small Angle Scattering (SAXS)

25. *Diffraction Anomalous Fine Structure (DAFS)*, I. Arcon et al., Jozef Stefan Institute, Ljubljana
26. *Determination of Gel and Aerogel Microstructure with Synchrotron Radiation,* A. Zidansek et al., Jozef Stefan Institute, Ljubljana
27. *X-ray Study of the Phase Transitions in Antiferoelectric Liquid Crystal,* R. Blinc et al., Jozef Stefan Institute, Ljubljana
28. *Structural Investigation of Bio- and Synthetic Polymers in Solution,* A. Jamnik et al., Department of Chemistry, University of Ljubljana, Ljubljana
29. *Liquid Crystalline Polyurethane Ionomers*, T. Malavasic et al., National Institute of Chemistry, Ljubljana

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