MOBILITY MISSION REPORT

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MISSION TITLE

1st Greek Summer School Snychrotron Radiation: properties & applications

DESCRIPTION

Concerned organisations

Research entities

Concerned infrastructures or facilities

Other relevant infrastructure or facility to be specified

Concerned phases

Phase 2: Site characterisation

Themes and topics

Theme 2: Radioactive waste characterisation, processing and storage (Pre-disposal activities), and source term understanding for disposal

- Waste handling, characterisation, treatment and packaging
- Interim storage
- Transportation between facilities
- Radionuclide inventory and source term

- Theme 5: Geological disposal facility design and the practicalities of construction, operations and closure
    - Facility and disposal system design
    - Constructability, demonstration and verification testing
    - Health and safety during transport, construction, operations and closure
    - Monitoring and retrievability
- Theme 7: Performance assessment, safety case development, and safety analyses
    - Integration of safety-related information
    - Performance assessment and system models
    - Treatment of uncertainties

Keywords

Synchrotron Radiation Instrumentation; Powder Synchrotron X-ray Diffraction; X-ray Imaging and tomography; XANES; EXAFS

EXECUTIVE SUMMARY

The program consists of hour-long lectures and afternoon Lab courses where the participants had the opportunity to handle experimental data and practice on data evaluation and visualization (infographics). The tutors are experts in the field of Synchrotron Radiation. One of our future plans is to perform further synchrotron XRD and X-ray absorption measurements on borosilicate glass samples which matrix elements include Si, B, Na, Ba and Zr, other additions include Ce, Nd, Eu and U to observe the fine structure of borosilicate glasses better and understand the effects of actinide and lanthanide addition to a glass matrix. I have already had the opportunity to learn a number of techniques (XANES, EXAFS, GIXRF) through my studies and have been able to participate in synchrotron measurements at Elettra, I would like to further expand my knowledge on the subject and acquire the knowledge needed to evaluate and analyse the data. During the summer school we had hour-long lectures and afternoon Lab courses where we had the opportunity to handle experimental data and practice on data evolution and visualization. The program lasted four days, each day had a different main topic and theme. On the first day, we studied the principals of synchrotron radiation, which included the properties of the beamline as well as the overall structure of a facility and its instrumentation. On the following day, we studied X-ray diffraction, which can be performed both on powder samples and on single crystals, and in the rest of the day, we also studied X-ray scattering, which was connected to a laboratory exercise, so we got to know the use of FullProf, GSAS-II, VESTA and PowDLL programs. After that, X-ray spectroscopy was the main topic. In this section we learned about X-ray absorption fine structure, X-ray Fluorescene, high resolution X-ray spectroscopy and X-ray Magnetic Circular Dichroism and their implementation in material science. During the lab course, we learned to use ATHENA and ARTEMIS from the Demeter software packages to evaluate and process real-life data and we used the PyMca program to analyze and quantify Sy-XRF spectrums. The last day was about X-ray imaging, mainly Scanning X-ray microscopy and X-ray tomography. We also studied some extreme conditions/industrial applications regarding this topic. My final conclusion about the summer school is that it was incredibly important to further expand my knowledge on this subject. The presentations were given by experts, who helped me to get the most up-to-date information possible regarding synchrotron radiation. The lectures and lab courses on EXAFS, XANES and X-ray tomography are essential so that I can evaluate similar data in my PhD thesis in the most precise way.

1. MISSION BACKGROUND

1.1. R&D background

The program consists of hour-long lectures and afternoon Lab courses where the participants will have the opportunity to handle experimental data and practice on data evaluation and visualization (infographics). The tutors are experts in the field of Synchrotron Radiation.

1.2. Mission objectives

One of our future plans is to perform further synchrotron XRD and X-ray absorption measurements on borosilicate glass samples which matrix elements include Si, B, Na, Ba and Zr, other additions include Ce, Nd, Eu and U to observe the fine structure of borosilicate glasses better and understand the effects of actinide and lanthanide addition to a glass matrix. Although I have already had the opportunity to learn a number of techniques (XANES, EXAFS, GIXRF) through my studies and have been able to participate in synchrotron measurements at Elettra, I would like to further expand my knowledge on the subject and acquire the knowledge needed to evaluate the data.

1.3. Mission request

I am very confident that this training opportunity can provide this, so I would be grateful if the Committee could provide financial support through the mobility program.

1.4. Mission composition

Host organisation

Aristotle University of Thessaloniki

Host facility

KEDEK AUTH – Balkan Center, Building A and B

Mission dates

4 September 2022 – 10 September 2022

2. MAJOR PRACTICES, TECHNIQUES, METHODS, TOOLS OR SYSTEMS OPERATED OR STUDIED

2.1. Practice, technique, method, tool or system operated or studied during the mission

Synchrotron X-ray Diffraction

Description

Application of synchrotron X-ray diffraction on powder and single crystal.

Usage

We learned the benefits of using synchrotron light for X-ray diffraction measurements. We understood the basics of the technique, how it can be used for powder samples and single crystals. In addition to the steps of data collection, we also studied data analysis.

Benefits

Having a better understanding of the technique and the overall data analysis regarding the data scaling, reduction and correction. I also have more knowledge on how to choose the adequate sample and beamline for the measurements. We currently have an application under evaluation at the Synchrotron SOLEIL, after a successful application and measurement, I will be able to evaluate the results of the borosilicate glasses.

Limitations

The lecture and lab course were adequate for understanding the theoretical background, but more time is needed to fully understand and interpret the mathematical models.

Applicability

The use of X-ray diffraction is preferable for heavier elements, so it can be beneficial in the case of our samples in which heavier elements are also present, such as U, Ce, Nd, Eu. I will know the method and I will be able to apply the acquired knowledge.

2.2. Practice, technique, method, tool or system operated or studied during the mission

XAFS spectroscopies

Description

Getting acquainted with Demeter software packages, experimental data processing and analysis.

Usage

ATHENA is an interactive graphical utility for processing EXAFS data, i.e. convert raw data to μ(E), fit linear combinations of standards to μ(E), perform background removal and execute forward and backward Fourier transformations.

Benefits

During the lab exercise, we learned to use its features and worked with real life data. In the future, I will be able to process and evaluate synchrotron data.

Limitations

We also studied FEFF code which is an automated program for ab initio multiple scattering calculations and yields scattering amplitudes and phases used in XAFS analysis. More time is needed to fully understand such a complex code.

Applicability

The knowledge acquired here is essential for me to be able to evaluate the results of synchrotron measurements carried out on our borosilicate glass samples in the future.

2.3. Practice, technique, method, tool or system operated or studied during the mission

Description

Usage

Benefits

Limitations

Applicability

2.4. Practice, technique, method, tool or system operated or studied during the mission

Description

Usage

Benefits

Limitations

Applicability

3. MISSION FINDINGS AND CONCLUSIONS

3.1. Lessons learned and conclusions

During the summer school we had hour-long lectures and afternoon Lab courses where we had the opportunity to handle experimental data and practice on data evolution and visualization. The program lasted four days, each day had a different main topic and theme. On the first day, we studied the principals of synchrotron radiation, which included the properties of the beamline as well as the overall structure of a facility and its instrumentation. On the following day, we studied X-ray diffraction, which can be performed both on powder samples and on single crystals, and in the rest of the day, we also studied X-ray scattering, which was connected to a laboratory exercise, so we got to know the use of FullProf, GSAS-II, VESTA and PowDLL programs. After that, X-ray spectroscopy was the main topic. In this section we learned about X-ray absorption fine structure, X-ray Fluorescene, high resolution X-ray spectroscopy and X-ray Magnetic Circular Dichroism and their implementation in material science. During the lab course, we learned to use ATHENA and ARTEMIS from the Demeter software packages to evaluate and process real-life data and we used the PyMca program to analyze and quantify Sy-XRF spectrums. The last day was about X-ray imaging, mainly Scanning X-ray microscopy and X-ray tomography. We also studied some extreme conditions/industrial applications regarding this topic. My final conclusion about the summer school is that it was incredibly important to further expand my knowledge on this subject. The presentations were given by experts, who helped me to get the most up-to-date information possible regarding synchrotron radiation. The lectures and lab courses on EXAFS, XANES and X-ray tomography are essential so that I can evaluate similar data in my PhD thesis in the most precise way.

3.2. Relevant findings and conclusions for home organisation

3.3. Relevant findings and conclusions for host organisation

3.4. Relevant findings and conclusions for other organisations

4. POTENTIALS FOR IMPROVEMENT OR DEVELOPMENT

4.1. Generic potentials

I was very satisfied with the summer school. Its organization and the quality of the presentations were excellent. In addition to the lectures, we had the opportunity to talk with our peers, and discuss professional topics. My suggestion would be to promote the event better, so it can reach more foreign students.

4.2. Potentials for home organisation

4.3. Potentials for host organisation

APPENDICES

Mission journal

DAY-1

I have participated in five hour-long lectures namely Synchrotons and ESRF; Accelerator Physics for Synchrotron Light Users; X-ray optics and beamlines; Synchrotron Radiation Instrumentation and Free Electron Lasers: principles and selected applications. In the afternoon, during the lab course, I worked with a software package called McXtrace which is a tool for carrying out highly complex Monte Carlo ray-tracing simulations of X-ray beamlines to high precision. In the evening, a get-to-know party was organized in which I participated, so I could get to know the research of the other students.

DAY-2

I have participated in five hour-long lectures namely Powder and Single Crystal Synchrotron X-ray Diffraction; Introduction to macromolecular crystallography; Small angle X-ray Scattering from macromolecular systems; X-ray total scattering in Materials Science; X-ray protein crystallography – challenges and opportunities from sample preparation to 3D structure determination. During the lab course, I used known platforms to prepare instruction files and refine data from polycrystalline materials obtained from a synchrotron source by applying Rietveld method. The lift of the used softwares are FullProf, GSAS-II, VESTA and PowDLL.

DAY-3

I have participated in four hour-long lectures namely X-ray absorption fine structure spectroscopies for study of matter; X-ray Fluorescence; An Introduction to high resolution X-ray spectroscopy and energy-science applications; X-ray Magnetic Circular Dichroism on ultra-thin layers. During the lab course, I got acquainted with processing and analysis of EXAFS data using Demeter, which included ATHENA and FEFF code, I also got acquainted with the qualitative and quantitative analysis of XRF data using PyMca.

DAY-4

I have participated in four hour-long lectures namely Scanning X-ray microscopies at the ESRF: a synergy between imaging and chemistry; X-ray tomography; Inelastic X-ray scattering: technique and sample environments; The European Synchrotron: a knowledge hub for industry. During the lab course I used the ROI imaging toll of PyMca and covered the topic of simple region of interest imaging; the use of clustering techniques; the batch treatment of fluorescence spectra and the applications to other synchrotron techniques. I also had the opportunity to get acquainted with the processing and analysis of synchrotron x-ray phase contrast imaging data using TomoPy and other open source python image processing libraries such as ITK.

Mission bibliography

MISSION BENEFICIARY

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PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

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Home organisation experts

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REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
2022.09.23	Istvan Tolnai	Margit Fabian	Fani Pinakidou