MOBILITY MISSION REPORT

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MISSION TITLE

Participation at the First Greek Summer School on Synchrotron Radiation:properties and 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 4: Geoscience to understand rock properties, radionuclide transport and long-term geological evolution

- Long-term stability (uplift, erosion and tectonics)

    - Perturbations (gas, temperature and chemistry)
    - Aqueous pathways and radionuclide migration
- 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

material science; application of synchrotron radiation; characterization of uptake by clay minearls; EXAFS; XANES

EXECUTIVE SUMMARY

My main research topic is to study the uptake and diffusion properties of different radionuclides. In our research in some cases synchrotron radiation is needed to be applied for two main reasons: (i) the concentration of analytes could be very low so that a laboratory equipment is not applicable, (ii) for certain analytical techniques (XANES, EXAFS) a tunable excitation energy is needed. To get familiar with new analytical methods and to have a better insight on the evaluation of X-ray absorption spectroscopy (XAS) this summer school looked a nice opportunity. During the 4-day long school 18 lectures (several of them were given by beamline scientists) and 6 lab courses were held. I had insight in the instrumentation of synchrotron facilities, on the possible X-ray optics and the fundamentals of the accelerator physics. Many X-ray scattering and diffraction lectures were given in connection to the lab courses where the evaluation for crystallogprahy were demonstrated. In my day-to-day life I apply X-ray fluorescence (XRF) for measuring both solid and liquid phase samples. To evaluate the XRF spectra I apply PyMCA software which is very complex and powerful tool. Two of the lab courses were dedicated to the application of PyMCA at different fields, these presentations were given by the developer of this software. A very nice presentation of XAS and a subsequetive practice were held where we had the opportunity to see how EXAFS spectrum are evaluated and how simulations are run. Thanks to the knowledge I gathered in this summer school in the future I will be able to try to interpret EXAFS results and come up with new ideas how to setup a beamline for our experiments.

1. MISSION BACKGROUND

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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 real experimental data and practice on data evaluation and visualization (infographics). The tutors are experts in the field of Synchrotron Radiation.

1.2. Mission objectives

My prospects for this summer school are to have a better understanding of EXAFS and XRD studies at synchrotron and therefore moving forward the evaluation process of our acquired data.

1.3. Mission request

I was wondering and I would be extremely thankful if the Committee could provide me financial support through the Mobility program for widening my capabilities of synchrotron studies.

1.4. Mission composition

Host organisation

Aristotle University of Thessaloniki

Host facility

Faculty of sciences, school of physics

Mission dates

4 September 2022 – 10 September 2022

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

Klikněte nebo klepněte sem a zadejte text.

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

X-ray optics and beamlines

Description

X-Ray Optical Elements and Beamlines for Science at Synchrotron- and FEL-Sources

Usage

We had a ray tracing practice with McXtrace where we applied the gathered knowledge from previous lectures

Benefits

I have an overview on the possible optical elements which can be applied at a beamline during my experiment

Limitations

We did not have the possibility to try out these different X-ray optical elements in real life

Applicability

I have some new idea to implement at our custom built micro-XRF instrument

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

X-ray absorption fine structure spectroscopies for the study of matter

Description

We studied the basic principles of XAS and the different acquisition modes, looked through what influences the EXAFS region and the XANES region of X-ray absorption spectrum.

Usage

We applied Athena software to normalize the spectrum and to transfer the collected data to k-space.

Benefits

I studied some new features of Athena software and I understand better spectrum acquisition techniques.

Limitations

Probably more times were needed to show in more detail the avaluation of EXAFS.

Applicability

To study the oxidation state of the sorbed selenium on argillaceous minerals.

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

Sy-XRF: spectrum analysis and quantification

Description

This Lab Course dealt with the qualitative and quantitative analysis of XRF data

Usage

Qualitative and quantitative analysis of XRF spectra with PyMCA

Benefits

Having a better application of data input, spectra calibration, peak identification and quantitative analysis

Limitations

For the deeper explanation of fundamental parameters of the configuration file much more time were needed

Applicability

I will be able to perform my batch fittings of my XRF maps considerably faster

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

I had insight in the instrumentation of synchrotron facilities, on the possible X-ray optics and the fundamentals of the accelerator physics. Many X-ray scattering and diffraction lectures were given in connection to the lab courses where the evaluation for crystallogprahy were demonstrated. In my day-to-day life I apply X-ray fluorescence (XRF) for measuring both solid and liquid phase samples. To evaluate the XRF spectra I apply PyMCA software which is very complex and powerful tool. Two of the lab courses were dedicated to the application of PyMCA at different fields , these presentations were given by the developer of this software. A very nice presentation of X-ray absorption spectrometry and a subsequetive practice were held where we had the opportunity to see how extended X-ray absorption fine structure (EXAFS) spectrum are evaluated and how simulations are run. In the future we plan to perform micro X-ray absorption near edge structure and EXAFS to study the chemical state of sorbed selenium to argillaceous rocks. In my point of view the bigger obstacle of EXAFS is not to measure but to evaluate. During the summer school I studied the foundation of EXAFS assessment. For simulation of EXAFS the parameters required by FEFF code could be easily obtained via Athena software. Special attention need to be paid of the Debye-Waller factors in the view of the thermal component. Even though the high inhomogenity of clayish systems, the components belong to the nanoscale which could alter the coordination number. Nevertheless the complex matrix EXAFS is such a powerful tool that it could provide average coordination number of the element of interest in our study.

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

4.2. Potentials for home organisation

4.3. Potentials for host organisation

APPENDICES

Mission journal

4 September 2022 – Travelling from Szombathely (Hungary) to Wien (Asutria) by train and then fly to Thessaloniki. Arriving in Greece around 11 and then taking a taxi to Metropolitan Hotel

5 September 2022- Getting to the venue and registration in the morning until 9 AM. Then participate lectures and lab courses until 8 PM about accelerator physics, synchrotron radiation instrumentation and X-ray optics. A dinner was organised at the university.

6 September 2022- Lectures and lab courses between 9 AM – 8 PM about X-ray diffraction, crystallography and differenc scattering methods

7 September 2022 - Lectures and lab courses between 9 AM – 8 PM about X-ray absorption spectroscopy, XRF spectroscopy and high resolution X-ray spectroscopy and a very nice lab course of XANES and EXAFS

8 September 2022 - Lectures and lab courses between 9 AM – 8 PM about X-ray tomography, imaging techniques and industrial collaborations at the ESRF

9 September 2022 – Taking a flight from Thessaloniki TO Wien. Since the flight was delayed we missed our last bus to Budapest, so we stayed at Wien during the night and departing to Hungary the next morning

10 September 2022 – Departing to Budapest with train around 10 AM.

Mission bibliography

MISSION BENEFICIARY

Ottó Czömpöly
PhD student
Environmental Physics Laboratory
Centre for Energy Research

PARTNER EXPERTS CONTRIBUTING TO THE MISSION

Host organisation experts

- Prof. Maria Katsikini, Aristotle Univ. of Thessaloniki
- Prof. Eleni C. Paloura, Aristotle Univ. of Thessaloniki
- Dr. F. Pinakidou, Aristotle Univ. of Thessaloniki
- Prof. Makis Angelakeris, Aristotle Univ. of Thessaloniki

Home organisation experts

- Dr. János Osán, Centre for Energy Research
- Dr. Margit Fábián, Centre fore Energy Research

Other organisations experts

- Dr. Andreas-Germanos Karydas, NCSR "Demokritos"
- Dr. Alexandros Lappas, FORTH
- Dr. Thanos Papazoglou, ESRF

REPORT APPROVAL

Date	Beneficiary	Home mentor/supervisor	Host mentor/supervisor
2022.09.15	Ottó Czömpöly	Dr. Osán János	Dr. Fani Pinakidou
	Visa	Visa	Visa