Synchrotron Radiation Center MAX IV Lab and Opportunities for Estonian Researchers

Marco Kirm, Vambola Kisand and Rainer Pärna
Synchrotron radiation

Radiation generated by accelerated high energy electrons moving in a magnetic field

Synchrotron facility MAX IV

Bending magnet radiation

Crab Nebula

Radiation produced by electron in magnetic field of neutron star
MAX IV laboratory and ESS

Sweden

Denmark

Lund

Estonia

Latvia

Lithuania
SR Applications

**High spatial resolution** (< a few nanometer)

**Time resolved studies** (< femtoseconds $10^{-15}$ s)

**High chemical sensitivity** (dilute samples or detailed electronic structure)

**Collimated beam** -> complex structures

**Coherence** -> new possibilities for X-ray imaging

Nano engineering
Electronics
Fibers
Composites
Micro-fluidics

Phase transitions
Catalysts
Energy storage
Photo-biology

Environmental Sc.
Films and interfaces
Gases
Superconductors
Magnetism

Pharmacy (Proteins/ viruses)
Polymers
Cellulose

Metallurgy
Medicine
**The MAX IV Accelerators**

300 m 3.x GeV LINAC: Injects the rings & Drives femtosecond X-ray source

1.5 GeV ring (96 m)
- 12 straights
- 5.6 nm rad horz emitt
- Current performance: 250 mA top-up operation
- 500 mA / 3 Ah studies

3.0 GeV ring (528 m)
- 20 straights
- 0.24 nm rad (hor)
- Current performance: 0.34 nm rad measured
- 250 mA top-up operation
- 380 mA studies
- Orbit stability below 10%

Commissioning and first-year operational results of the MAX IV 3 GeV ring

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545 m
The 16 funded beamlines, 11 of those using SR light

1. FemtoMAX
   - Ultra-fast processes in materials
2. NanoMAX
   - Imaging, spectroscopic & scattering with nanometer resolution
3. BALDER
   - X-ray absorption spectroscopy in-situ and time resolve
4. BioMAX
   - Highly automated macromolecular crystallography
5. VERITAS
   - RIXS with unique resolving power and momentum resolution
6. HIPPIE
   - High-pressure photoelectron spectroscopy
7. BLOCH
   - Angle resolved photoelectron spectroscopy
8. FinEstBeAMS
   - Estonian-Finnish Beamline for Atmospheric & Materials Science
9. SPECIES
   - VUV High-pressure photoelectron spectroscopy and RIXS
10. FlexPES
    - Photoelectron Spectroscopy and NEXAFS
11. MAXPeem
    - Photoelectron microscopy
12. CoSAXS
    - Small angle scatter
13. SoftiMAX
    - Coherent Soft X-Ray Scattering, Holography
14. DanMAX
    - Paper and pulp
15. MicroMAX
    - Frontier MX
16. ForMAX
    - Paper and pulp
SR Techniques

**Scattering Beamlines** *(Structural Information)*
- e.g. Diffraction (single crystal/powder)
- Small Angle X-ray Scattering (SAXS)

**Spectroscopy beamlines** *(Chemical Information)*
- e.g. RIXS - Resonant Inelastic Scattering
- EXAFS - Extended X-ray absorption fine structure
- XPS - X-ray Photoelectron Spectroscopy

**Imaging beamlines** *(Dimensional geometrical or electronic structure or chemical composition)*
- e.g. Radiography (2D), Tomography (3D)
- CDI, PEEM
2, 3 or 4 – Dimensional geometrical or electronic structure or chemical composition
BioMAX (operating since 2017)

BioMAX is the first X-ray macromolecular crystallography beamline

X-ray beam focus is $20 \times 5 \mu m^2$

$2 \times 10^{13}$ ph/s at 500 mA

X-ray crystallography using microcrystals and ultra large unit cells
FinEstBeAMS

• 1st Internationally funded beam-line at MAX IV Lab
• A consortium of **Estonian and Finish Universities:**
University of Tartu, University of Oulu, University of Turku, University of Tampere

**Funding (initial investment 3.5+3.5 M€):**
European Regional Development Fund through Archimedes Foundation (Estonia), University of Tartu, Estonian Ministry of Education and Research
Academy of Finland
MAX IV Lab

3 + 1 Universities from Finland and Estonia
Grazing Incidence EPU BL – FinEstBeAMS with 3
elements

FinEstBEAMS

Undulator scanned synchronously with mono

What we can do with VUV-XUV radiation delivered by the FinEstBeaMS beamline?

Gas-phase endstation for spectroscopy
- Ion spectrometer
- Electron spectrometer
- $e^-$ Auger
- $h\nu$
- $e^-$
- $M_2^+$
- Photo luminescence endstation
- $h\nu_2$
- $M_1^+$
- $e^-$ Auger
- $h\nu$
- Solid state endstation
- Surfaces and interfaces
- CaWO$_4$
- Luminescence Scintillators
- Fragmentation of biomolecules, study of free molecules and clusters, ionic liquids – i.e. low density matter

What we can do with VUV-XUV radiation delivered by the FinEstBeaMS beamline?
BaF$_2$ cross-luminescence at FinEstBeAMS

Blue dots and reflection spectrum of BaF$_2$ – Kirm et al., SUPERLUMI HASYLAB 2002
The electronic structure of ionic liquids based on the TFSI anion: A gas phase UPS and DFT study

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ABSTRACT

The valence bands of [EMIM][TFSI], [DEME][TFSI] and [PYR14][TFSI] gas-phase ion pairs have been investigated using ultraviolet photoelectron spectroscopy (UPS). The photoelectron spectra are interpreted by using several density functional and ab initio calculation methods. Although the experimental vapor phase spectra are similar, the different calculation methods make different predictions about the HOMO molecular state of the ion-pairs of the ionic liquids. The HOMO state of the [DEME][TFSI] ion-pair is due to the TFSI anion, while in [EMIM][TFSI] it is due to the EMIM cation. However, it is difficult to make conclusive assignments for the [PYR14][TFSI] ionic liquid. All calculation methods predict the LUMO to be of cationic origin in all the studied ion-pairs.
BENEFITS of INVESTMENT INTO FinEsTBeAMS

- Our researchers get access to large scale infrastructures, which will be never realized in Estonia.
- Large scale facilities acts as catalysts bringing together researchers from various fields, interdisciplinary ideas and creating breakthrough solutions in technology areas – networking.
- Investments into the FinEstBeAMS will grant Estonian research community (academic and industrial) competition free access to any beamline at MAX IV Lab. In addition to that regular beamtime calls reviewed according to their scientific quality are free to apply.
FUTURE of FinEstBeAMS

Research, Research, Research - national and International cooperation

Estonian RI ROADMAP funding delivered MAX-TEENUS (01.10.2020):
- to develop FinEsTBeAMS equipment (endstations) further;
- training of Estonian Users and Providing on-site Support.

NEW USERS from ACADEMIA and Industry

Creation of Estonian Users Organisation - Universities, Institutes, Industry
Aitäh!

A photoluminescence endstation at FinEstBeAMS 1.5 GeV ring at MAX IV Lab Lund, Sweden

1st scheduled commissioning beamtime

October 2018
Photo Ivo Romet
Thank you for FinEsTBeAMS

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Prof. Ergo Nõmmiste, Tartu Ülikool
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