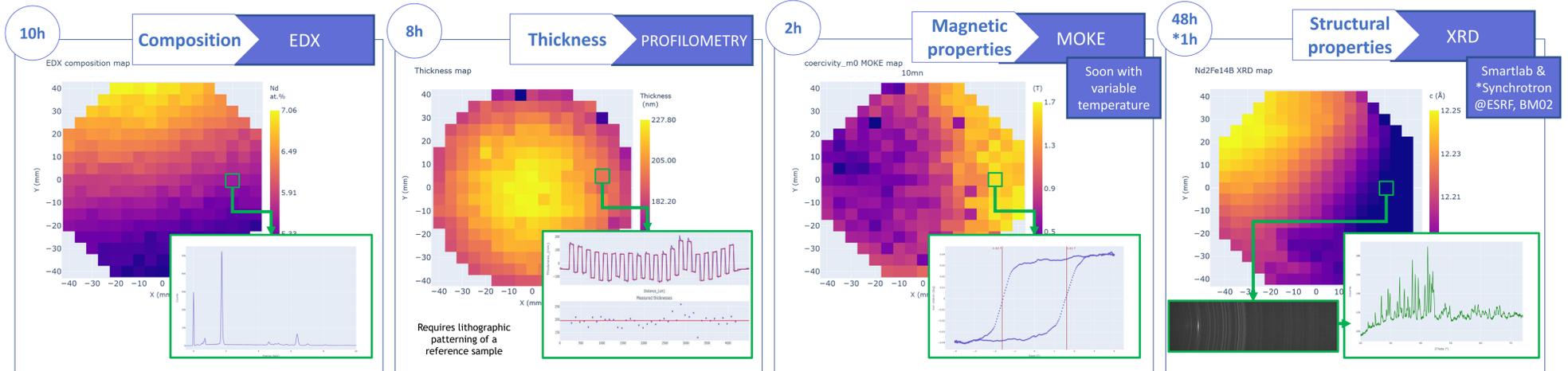
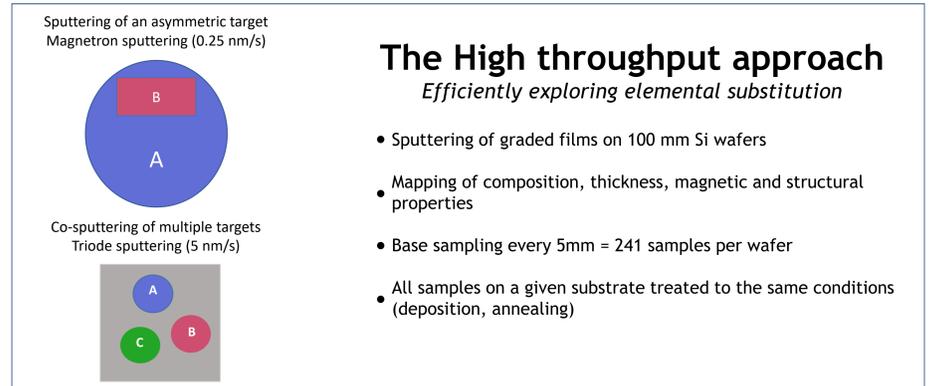
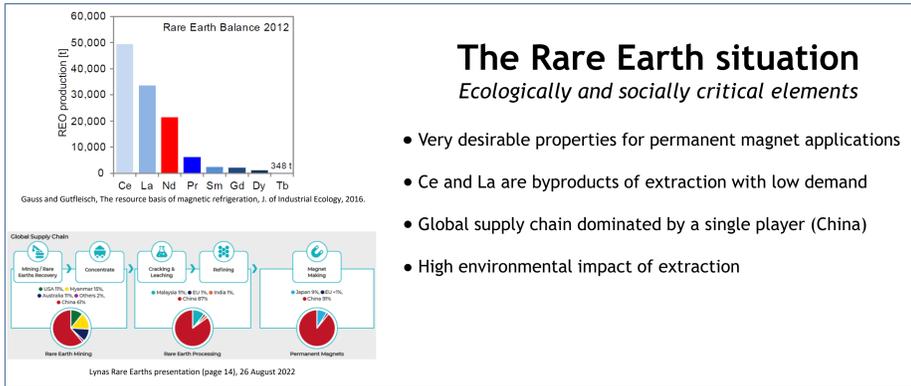


# Development of data handling tools for high-throughput experiments Towards sustainable magnets

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Permanent magnets are at the center of current efforts to decarbonize society. From windmills to electric motors, our current plan for reducing greenhouse gas emissions will require a large amount of high performance magnets, and by extension, rare-earth metals. Unfortunately, rare earth metals are stuck in a complex ecological and geopolitical context, and the future of supply is uncertain. In an effort to reduce consumption of the most critical rare earth elements in known materials and optimize alternatives, we are developing a high throughput approach to quickly evaluate the effects of elemental substitution in hard magnetic materials.



Our high throughput experiments quickly generate large, convoluted datasets. In order to organize and extract trends from these measurements in a timely manner, specialized tools are needed. To simplify data storage and sharing, an **HDF5 based file system** has been developed. In order to interface with these HDF5 files and the data within, a **dedicated python software & user interface** has been developed. All software is open source, and has been developed with FAIR data principles in mind (Findable, Accessible, Interoperable, Reusable).



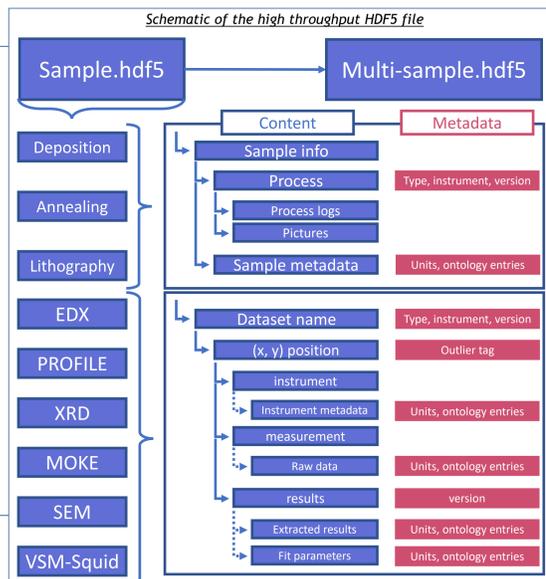
## Hierarchical Data Format

Modern and flexible file format

- Free, Open source, non-profit organization
- Heterogeneous data in a homogeneous file
- Metadata inextricably linked with data
- Accommodates big datasets
- Widely adopted by institutions and research teams worldwide (ex: NeXUS)
- Strong community with many tools already developed



<https://www.hdfgroup.org/>



## High Throughput HDF5:

File structure tailored to our specific needs

- All relevant datasets for a system with a single file
- Rich metadata ensures information is always available
- Data treatment parameters and raw data kept with results
- Homogenization of different characterization methods
- Filter out proprietary file formats
- Simplify integration of multiple datasets
- Properly defined physical quantities through the Magnetic Materials Ontology [1] (MaMMoS)
- Easy sharing of data with partners

[1] <https://mammos-project.github.io/MagneticMaterialsOntology>



## The Plotly - Dash ecosystem

Python data apps with web interface

- Free, Open source (MIT license)
- 100% Python (and maybe a bit of CSS)
- Many community developed and maintained modules

[dash.plotly.com](https://dash.plotly.com)

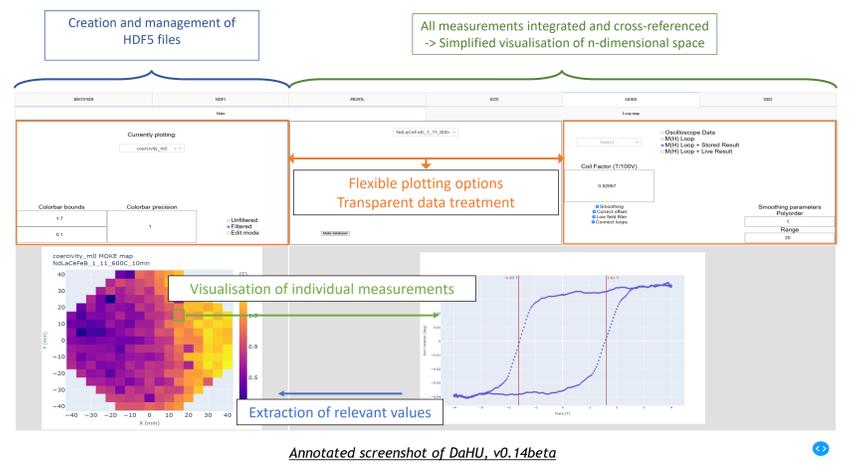


## Dash High throughput Utilities (DaHU)

Our pipeline for data handling

- Create and manage high throughput HDF5 files and datasets
- Treat and fit data
- Save and document calibration measurements
- Visualize heatmaps and individual measurements
- Export HDF5 to CSV for compatibility

<https://github.com/Combinatorials-Neel/DaHU>



Our high throughput suite for the study of magnetic materials is fully functional, generating volumes of valuable data, and tools are being developed to speed up analysis. So far, we have been focusing on conventional data treatment methods, but we are now exploring possibilities to apply machine learning techniques to help extract additional information and spot trends. The high throughput toolbox is also expanding, with microstructure imaging and variable temperature MOKE currently being developed, which will add more dimensions to our datasets and strengthen the need for appropriate data handling solutions. With clean and comprehensive data, we hope to be able to guide the development of future magnets.

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