Moving towards fully Open Data for Reflectometry

The move towards open science continues to gather pace and is becoming well established at central facilities. The situation is less clear for X-ray reflectometry studies conducted in home laboratories. In this session, we review the current landscape and present the latest from the Photon and Neutron Open Science Cluster (PaNOSC) and discuss how we can leverage these developments within the Reflectometry community. We will also explore data catalogues and data support and hold an open discussion to facilitate a gap analysis of needs.

Tim Wetzel: 'A catalogue concept for FAIR and Open Data implemented at DESY for NFDI and EOSC.'
Tom Hase: 'The new UK Physical Sciences Data Infrastructure project and how we can exploit it'
Open discussion on moving towards open data (focus on metadata needs): Moderated by Bridget Murphy:

- 1. Cataloguing reflectometry data
 - Importance of inter-operability and consistent ontologies/metadata
 - Need for federalised architectures to facilitate searches.
 - SciCat: open repository for central facility and lab-based data with ORSO based metadata capture
 - Possible to have localised repositories (facility/university/group level)
 - Multiple options, but strong push for ORSO to endorse <u>SciCat for reflectometry</u>

Metadata

- What data to collect and how to flag "good" or "bad" data
- Dangers and over-reliance on automatically generated tools, especially for sample details
- Need for flexibility
- Ontology/schema evolution based on community and international standards

3. Training:

- Awareness raising approaches at different levels.
- Upskilling and lack of user knowledge
- Education (from metadata needs to workflows/pathways and then to machine learning)
- Recognising the "people" in the process

Useful Web-links

- SciCat
- DAPHNE4NFDI
- PSDI
- •FAIR data the photon and neutron communities move together towards open science
- •Snip electronic lab book
- PaNOSC
- PAN-training
- EOSC nodes
- •NFDI