




# From Neutrons to Structure in Materials: Hands-On Introduction to Neutron Data Analysis

 17–18 November 2025  
 IFJ PAN, Kraków & Online  
 Hybrid Format

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## Day 1 – Instructions and tentative schedule

**Topic:** *Neutron Powder Diffraction – From Nuclear to Magnetic Structure Refinement*  
**Instructor:** Dr. Naveen Kumar Chogondahalli Muniraju (IFJ PAN, Kraków)

### Required software:

1. [Mag2Pol](#) (Navid Qureshi, ILL)
2. [Vesta](#) (Koichi Momma and Fujio Izumi, JP-Minerals)

Bookmark the following useful websites:

1. [Materials project \(signup for free!\)](#)
2. [Crystallography Open Database](#)
2. [Neutron activation and scattering calculator](#)
3. [Bilbao Crystallographic Server](#)

Time	Session	Description
10:00 – 10:15	Welcome & Introduction	Workshop overview and setup.
10:15 – 11:00	Session 1: Neutron Diffraction – Concepts and Applications	Brief introduction to neutron diffraction; discussion of experimental aspects and what structural information (nuclear, magnetic, diffuse) can be obtained from powder and single-crystal data; overview of proposal preparation.
11:00 – 11:45	Session 2: Guided Hands-On – Refinement of Lattice Structure from NPD data and Magnetic structure refinement - Setup	Step-by-step refinement of the nuclear (lattice) structure using a known dataset and setup of the magnetic structure. Participants follow along with live guidance. (Necessary software and data will be shared a few days in advance)
11:45 – 13:00	Lunch Break	
13:00 – 14:15	Session 3: Guided Hands-On – Magnetic Structure Refinement	Participants refine magnetic structures on the datasets provided with instructor support. Discussion of refinement strategy, symmetry constraints, and interpretation of magnetic parameters.
14:15-14:30	Coffee break	
14:30 – 15:15	Continuation of hands-on exercise. Wrap-Up & Q&A	Continuation of the hands-on refinement, summary of results, discussion, and Q&A.

## Day 2 – Instructions and tentative schedule

**Topic:** *Polarized Neutron Reflectometry – Modeling magnetic thin films and heterostructures*

**Instructor:** Dr. Artur Glavic (PSI Center for Neutron and Muon Instrumentation, Switzerland)

### Required software:

1. [GenX 3](#) (Artur Glavic, PSI), please install and test in advance, see the [documentation](#) if you need help installing on your system.

Bookmark the following useful websites:

1. [Open Reflectometry Standards Organization](#)
2. [Scattering length density database](#) for looking up and calculating SLDs

Time	Session	Description
10:00 – 11:00	Session 1: Reflectometry basics, neutron polarization	Brief introduction to the x-ray and neutron reflectometry technique explaining how information about nano-scale structure in thin films and heterostructures can be gained. Using polarized neutrons this can be expanded to magnetic depth profiles.
11:00 – 11:45	Session 2: Introduction to reflectometry modeling	Building a model for reflectometry analysis using the GenX software. Parametrization of the model, defining layer structures, using the Software and running refinements.
11:45 – 13:00	Lunch Break	
13:00 – 14:00	Session 3: Hands-On Exercise in PNR analysis	The participants will be split into breakout rooms with a PNR dataset used in a relevant publication. The teams will try to fit the results with the Instructor jumping between groups to give regular support.
14:00-14:15	Coffee break	
14:15 – 15:15	Session 4: Estimating fit uncertainty. Short Wrap-Up & Q&A	General explanation about fitting routines and caveats. Using modern techniques to better understand parameter uncertainties.