Neutron Powder Diffraction

Investigation of crystal structures

Introduction

X-rays vs. Neutrons
For many decades X-ray powder diffraction (XRD) has been an established and versatile tool for manifold applications in material science and engineering. It is well known as a rapid analytical method, used for both routine examination and scientific characterization of crystalline materials.

Neutron powder diffraction in terms of its principles of operation is similar to X-ray diffraction. Contrary to X-rays, however, which interact primarily with the electron cloud surrounding each atom of a given material, most scattering of neutrons occurs at the atom nuclei, thus providing complementary information not accessible with X-rays.

The neutron furthermore carries a magnetic moment, which makes it an excellent probe for the determination of magnetic properties of matter.

In the majority of cases, diffraction is the main mechanism of the interaction of the neutron with matter. This is why powder diffraction experiments are perhaps the most straightforward among all neutron scattering techniques.

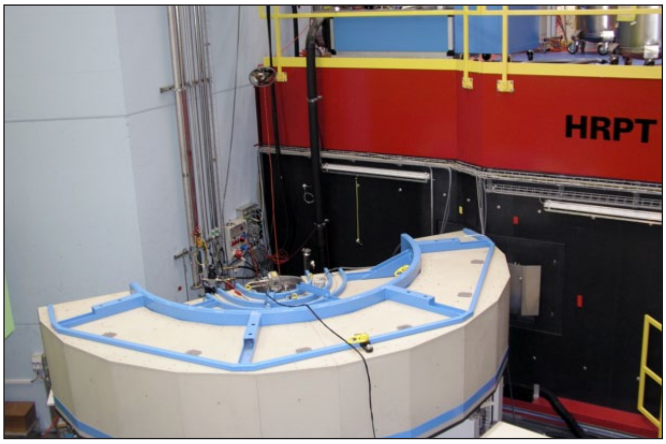

Figure 2: **HRPT: Powder diffractometer.**

The extracted information is in many cases unique compared to that obtained from conventional X-ray diffraction techniques, because neutrons are *sensitive to low atomic number materials,* such as Hydrogen and Boron, and capable of distinguishing between *elements with adjacent atomic numbers,* such as Iron and Cobalt, *Isotopes* of the same element, or *element groups whose atomic numbers are wide apart,* such as Palladium and Hydrogen (Deuterium). For these materials systems ,neutron powder diffraction is ideally suited to addressing the shortcomings of conventional XRD methods.

Physical properties gained

The most common information typically extracted from a neutron powder diffraction experiment includes the symmetry of crystal lattices, the dimensions of the unit cells of the crystal structures and the elemental composition thereof. Additionally, the fractional coordinates and occupation factors of the atoms within the unit cell are extracted with typically very high precision, providing reliable information on the interatomic bond distances, angles and thermal displacements of atoms.

Finally, microstructure parameters characterizing the grain size distributions and microstresses in the crystal lattice may also be determined.

Applications

Neutron powder diffraction is most widely used in the fields of crystallography, mineralogy, geochemistry, solid-state physics, chemistry, material science & engineering and biology. Some materials systems, specifically accessible and predestined to be

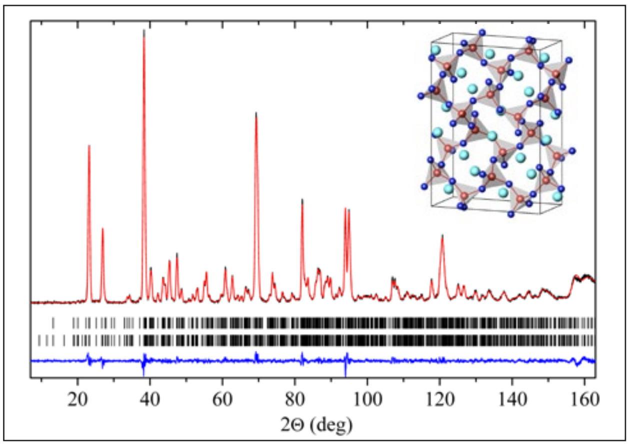

Figure 1: **Structual determination of orthorhombic $RbFeO_2$ – Rietveld refinement plot of the HRPT data collected at T=1.5K: both crystal and magnetic structure refinement.**

analyzed with this technique, are highlighted below:

- Metallic alloys
- Powdered minerals
- Ceramics
- Isotope-substituted materials
- Low atomic number materials
- Hydrogen storage materials
- Antiferromagnetic and ferromagnetic materials

Neutron powder diffractometers at SINQ

Neutron diffraction experiments are carried out using sophisticated modern instruments located at powerful neutron sources, such as nuclear reactors or spallation (accelerator-type) sources. Among other large-scale facilities, PSI operates the Swiss spallation neutron source SINQ[1], which encompasses an up-to-date park of neutron scattering instruments.

Among these, two neutron powder diffractometers, DMC[2] and HRPT[3], are highlighted below:

DMC

The high-intensity diffractometer DMC is mainly designed for studies of phase transitions and the detection of weak or fast processes. DMC provides:

- high intensity for weak scattering materials or small samples
- access to low scattering angles, needed for magnetic structure determination

HRPT

Complementary to DMC, the diffractometer HRPT is designed for high-resolution neutron powder diffraction studies with thermal neutrons.

HRPT provides:

- very high resolution over a large scattering angle range
- high suitability for advanced structural determination

The broad range of research topics investigated at DMC and HRPT is complemented by a large collection of sample environments, covering an extremely wide range of pressures and temperatures.

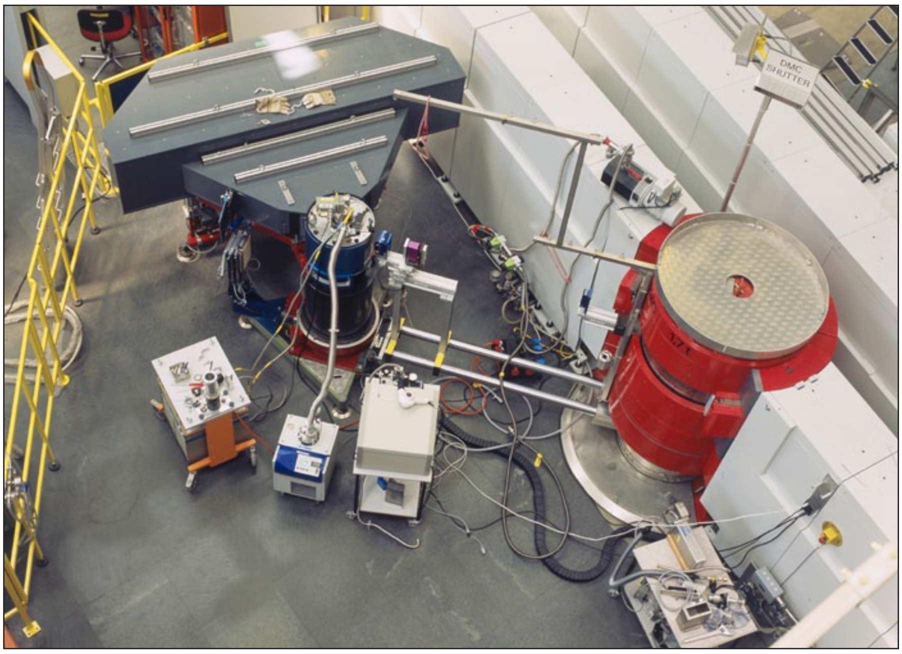

Figure 3: **The DMC powder diffractometer is also appropriate for the investigation of magnetic phenomena.**

The table below details the key operational characteristics of the DMC and HRPT instruments. Individual sample environment setups are possible on demand.

Properties	**DMC**	**HRPT**
Wavelength	2.3 – 6.0 Å	0.94 – 2.41 Å
Scattering range	80° (400 channels)	160° (1600 channels)
Best resolution Δd/d	≥ 0.006	≥ 0.0009
Temperature range, sample	110mK–1400 K (–273 °C …1127 °C)	
Magnetic field, sample	≤ 4 T (vertical), ≤ 2 T (horizontal)	
Hydrostatic pressure, sample	1.5 GPa (few cm^3), 10 GPa (few 10 mm^3)	
Beam size	Up to 5 cm (h) x 1 cm (w)	

Example

A typical HRPT diffraction pattern and the resulting crystal structure are shown in figure 1.

Contact us

Both, the HRPT and DMC diffractometers are open to users from the world-wide scientific community through the user-access program[4], as well as for scientific cooperation with industry.

Please feel free to ask us for further details.

[1] http://sinq.web.psi.ch/
[2] http://sinq.web.psi.ch/dmc
[3] http://sinq.web.psi.ch/hrpt
[4] https://duo.psi.ch/duo/, http://sinq.web.psi.ch/sinq/sinq_call.html

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