

Bragg Institute

2100 WOMBAT - High-Intensity Powder Diffractometer

Description

Materials with light elements in the presence of heavy ones (e.g. oxides, borides, carbides, etc.) can be measured with neutron powder diffraction, including magnetic materials. It is also a very useful technique for bulk samples or experiments in extreme environments (pressure, temperature, stress, magnetic and electric fields or combinations thereof). It is good for multiphase materials and for quantitative phase analysis, in which the presence of minority materials can be measured accurately.

WOMBAT high-*intensity* powder diffractometer. Its high performance comes from the combination of the best area detector ever constructed for neutron diffraction with the largest beam guide yet put into any research reactor and a correspondingly large crystal monochromator.

The method for achieving this is to build a flexible modular instrument which can exploit the advantages of (i) focussing neutron optics in the monochromator system over a wide range of incident wavelengths, (ii) a large solid angle detector with position sensitive detection capabilities, (iii) an advanced data acquisition electronics and (iv) a re-configurable collimation system which optimises the background reduction in each experiment.

Applications

WOMBAT is optimised for kinetics experiments and very small samples, and will specialise on *in-situ* studies of chemical reactions, other dynamic phenomena, high-pressure experiments and magnetism. Future scientific opportunities will likely include: novel hydrogen-storage materials, negative-thermal-expansion materials, methane-ice clathrates, pharmaceutical molecules, and materials for fusion reactors.

The mission for WOMBAT is to provide scientists with a high-intensity diffractometer at the OPAL reactor which can be used to carry out high-impact science in cases where

- the sample specimens are small (~10mg)
- the samples are contained in complex sample environment(s), for example in pressure cells
- rapid real time measurements are required to determine crystal structures quickly for phase transitions, chemical reactions and kinetic studies
- stroboscopic measurements are required on timescales down to 30 μ s

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Description

ECHIDNA is a high-*resolution* powder diffractometer optimised for structure determination of new materials. The instrument uses a single wavelength and a highly collimated neutron-beam to improve resolution. This diffraction technique can accurately resolve both complex atomic and magnetic structures. The high-resolution enables closely placed peaks in the diffraction pattern to be separated. This diffraction technique can accurately resolve both complex atomic and magnetic structures.

Applications

High-resolution powder diffraction can be used to:

- Determine structures of newly created materials, to better understand their properties.
- Study materials with light elements in the presence of heavy ones (e.g. oxides, borides, carbides) and for magnetic materials.
- Measure strain, crystallite size, and defects in materials such as metals, hydrogen storage and electro-chemical materials, and mesoscopic structures.
- Investigate materials that occur in a polycrystalline form under natural or industrial conditions.
- Investigate materials with complex crystal structures, including catalysts, hybrid materials, organics, cements, natural minerals, zeolites, and non-linear optical materials.
- Study the structural and magnetic phase transitions of ferroic and electronic materials such as superconductors and magnetoresistive materials.
- Investigate bulk samples or samples in extreme environments (pressure, temperature, stress, magnetic and electric fields, or combinations of these).

Relevant fields include:

Solid-state physics, materials science, chemistry, geoscience, and engineering.

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Description

Platypus is one of the world's top neutron reflectometers with the added ability of studying films at the air-liquid interface (free-liquid surfaces). Reflectometry is similar to small-angle scattering in the sense that it is sensitive to lengths on the nanoscale (between 1nm and 100nm), but it is done in reflection rather than transmission geometry. It contains interference information like that routinely seen, by eye, as the coloured sheen from oil films on water. Reflectometry is typically performed in a line geometry, rather than with pinholes. To get a good result, very perfect surfaces must be used, typically with depositions on commercial silicon wafers or other polished substrates (e.g. salt, quartz, glass, MgF₂, etc.). Free surfaces (e.g. a water or oil surface) can also be used, and special cells available to study solid-liquid interfaces (we have one). Experiments can be done under electrolytic action or shear. There is sometimes scattering away from the perfectly reflected specular beam, called diffuse scattering, and this contains quantitative information about the roughness of the surface(s) and about in-surface structure.

Reflectometry can be performed with both neutrons and X-rays: neutrons give different contrast, but are particularly suited for soft-matter systems in which H-D contrast variation is used, and magnetic materials using polarised neutrons and polarisation analysis.

Applications

Neutron reflectometry is used to study surfaces, thin films, buried interfaces, magnetic films, multi-layered structures and processes that occur at surfaces and interfaces. Neutron reflectometry provides information on the composition, changes in surface characteristics over time, thickness and interfacial roughness of thin films with the precision of a few atoms.

Neutron reflectometry can be used to:

- Study soft matter in biological and chemical science
- Deliver critical information about polymer film composition, chemical properties and the quality of the film in conjunction with other surface sensitive techniques.
- Study processes occurring at surfaces and interfaces such as adsorption, corrosion, adhesion and inter-diffusion between layers to solve important industrial problems
- Study thin-film magnetic devices to be used in future generations of computers, including magnetoresistive read head sensors and data storage films in hard drives as well as non-volatile magnetic random access memory devices.

Relevant fields include:

Biology, chemistry, surface engineering, magnetic memory.

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[PLATYPUS home page](#)

Description

In the Laue method of single-crystal diffraction, the crystal is illuminated by a very broad spectrum of wavelengths, and a large area of film is used to measure the arrangement of diffraction spots. The KOALA diffractometer uses a cylinder of image plates, arranged with the crystal at its centre. The broad-band radiation is provided by placing the instrument at an end-guide position.

Neutron single-crystal diffraction is absolutely essential (1) to determine the accurate positions of hydrogen atoms in solids, and (2) to determine the arrangements of magnetic moments in solids. In many cases, hydrogen positions can be inferred from the positions of the other (carbon, oxygen, nitrogen, etc.) atoms, but if *hydrogen bonding* occurs, this is not reliable. Many of the most important functions, e.g. in catalysis, pharmaceuticals and functional biology, depend on just such hydrogen bonds.

The diffraction patterns created when neutrons hit a sample in KOALA allow scientists to determine the location of atoms within the crystal and provide them with information about the crystal's structure and its properties. Single-crystal neutron diffraction studies complement X-ray crystallography by revealing the precise positions of light atoms such as hydrogen, which cannot be determined by X-ray.

KOALA, located on a thermal guide, is focussed on applications to small-molecule crystallography and materials science, but if the same instrument (or a similar one) were to be situated on a cold-neutron beam, it would be capable of tackling protein structures.

Applications

There are applications in a wide range of materials-science problems, including the new lightweight hydrogen-storage materials (alanates, metal-organic frameworks, etc.) that are under consideration for transportation applications as a substitute for hydrocarbons.

KOALA will be useful for:

- Development and study of new pharmaceuticals - through diffraction studies of potential drug candidates
- Modern synthetic chemistry research - using diffraction studies to fully determine specific interatomic interactions of new chemicals
- Advanced materials research - to identify materials and to examine subtly different formulations at the interatomic scale
- Minerals research - understanding of the structure of new phases and the effect of the different phases on processing conditions
- Distinguishing between iso-electronic species (eg. K⁺, Cl⁻ or elements near each other in the periodic table).

Relevant fields include: chemistry, physics, materials science, geology and biology.

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[KOALA home page](#)

Description

KOWARI is a residual stress diffractometer which can be used for 'strain scanning' of large engineering components as large as 1000 kilograms. The integrity of engineering components often depends on strains and stresses inside the material. For example, rails can fail if stresses exceed the 'ultimate tensile stress'. KOWARI is a non-destructive method applicable to nearly all crystalline materials which provides sub-surface information not obtainable by any other technique. It can determine important mechanical properties, to validate finite element models, which predict mechanical behaviour for increased reliable performance or lifetime predictions. It is also used to compare experimentally determined stresses with critical material characteristics. Mechanical strains and stresses can be revealed by measuring crystal lattice deformations with neutron diffraction. Neutrons are capable of penetrating deep into materials making them a unique tool to obtain data about lattice deformations deep inside the sample. 2- and 3-dimensional stress maps can be obtained by translating and rotating the object during the experiment.

The basic idea of strain scanning is to perform a diffraction experiment, and determine the lattice parameters for the phase(s) of interest in an engineering component. Deviations from a standard unstressed specimen (which can be another portion of the same object) are strains, and with some simple analysis stresses can be extracted. This may be averaged across a whole sample, for instance in the case of metal-ceramic composites, to understand how load is shared between the metal matrix and the ceramic reinforcement. More often, one uses carefully defined apertures before and after the specimen to define a gauge volume of $\sim 1\text{mm}^3$ or less. The object is then translated and rotated to map out the strains (and therefore the stresses) within the object of engineering interest.

The basic experiment is very simple, and the main challenge is to design the instrument sample table in such a way that it can accommodate large objects (up to 1 tonne) and move them around reproducibly to within ~ 20 mm.

The main advantage of using neutrons (as opposed to X-rays) is that neutrons can penetrate centimetres into the object of interest. X-rays, on the other hand, are mainly useful for surface problems, like coatings on gears or cutting tools, and for issues in the semiconductor industry. Both neutron and X-ray strain-scanning is limited to crystalline materials, so we cannot study stresses in plastics or glass by this method.

Applications

The KOWARI residual stress diffractometer can be used to reveal:

- Residual stresses in welds such as rails, pipelines, airplanes
- Stresses in coatings such as thermal barrier, wear resistant and corrosion resistant coatings
- Stress corrosion cracking due to extreme environments such as: heat + pressure (pressure pipes of power generators), corrosive environment + stress (pipelines, steel reinforcement in concrete)
- Fatigue, crack growth and development in materials undergoing contact stress, structural components and load-bearing parts.

In addition to its engineering applications, KOWARI can also be used to investigate new materials such as shape-memory alloys. These materials can return to their original shape after bending (e.g. vascular stents) or deformation and are used in medical and aerospace applications.

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[KOWARI home page](#)

Description

QUOKKA is a small-angle neutron scattering (SANS) instruments. SANS is a powerful technique for looking at sizes and structures of objects on the nanoscale (1-10nm), like polymer molecules, emulsions, colloids, defect structures in metals and ceramics, magnetic clusters, magnetic flux lines in type-II superconductors, porous materials, geological samples, alloys, and biological molecules such as proteins and membranes.

When a neutron beam impinges on a sample, some neutrons scatter along a path that differs from the transmitted beam by as little as several hundredths of a degree. This 'small-angle' scattering provides information about relatively large structural details on the nanoscale. SANS can provide particle sizes, shapes and distributions averaged over a complete macroscopic sample.

In many ways, small-angle scattering is complementary to electron microscopy while direct imaging is the domain of electron microscopy, SAXS and SANS can provide particle sizes, shapes and distributions averaged over a complete macroscopic sample. Small-angle scattering is rarely able to solve a problem on its own, and is typically used in conjunction with a number of other techniques.

Applications

The major strength of the SANS technique is that it can be used to investigate a host of materials, which cover a wide range of research disciplines. Materials that are routinely characterised using the SANS technique include: alloys, ceramics, biological materials, colloidal materials, complex fluids, polymers, surfaces and interfaces, flux lattices in superconductors. SANS is a versatile technique for investigating food components such as proteins, polymers and emulsions.

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2650 The Small Angle X-ray Scattering Instrument

Description

The SAXS instrument is a Bruker Nanostar equipped with a rotating anode source and three-pinhole collimation. SAXS is complimentary to Small Angle Neutron Scattering (SANS) which will be available on the new QUOKKA instrument at the OPAL research reactor. A variety of sample environments are available for solids and liquids, including two temperature control units one covering temperature range -30°C to 120°C and a second unit for ambient to 300°C. The instrument is capable of being run in two separate configurations either high resolution or high flux; the q-range accessible is 0.005 Å⁻¹ to 3.1 Å⁻¹ in high resolution mode and 0.01 Å⁻¹ to 3.1 Å⁻¹ in high flux mode.

Applications

SAXS is used to study any materials with structure of the length scale 1-100nm. The performance of many advanced materials is crucially dependent on nanostructure, and SAXS can be used to study this. It can be used for study of density variations, colloidal sizes, particles sizes, porosity, domain sizes, orientation, phase identification, the list is endless. With research being directed more towards nano-sized science, SAXS is becoming a widely used tool.



Instrument Specifications

Rotating Anode Cu Ka source (1.541 Å)
Cross-coupled Göbel mirrors
3 pinhole collimation
Large multifunctional sample chamber
Sample temperature control from -30°C to 150°C or ambient to 300°C
Hi-Star 2D detector with 100µm resolution
Capability of two configurations: high resolution or high intensity.
$Q_{\min} = 0.005 \text{ \AA}^{-1}$
$Q_{\max} = 3.1 \text{ \AA}^{-1}$

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[SAXS home page](#)

Description

TAIPAN is a triple-axis spectrometer used to measure neutron inelastic scattering, which is a key technique for the measurement of excitations in materials. These measurements provide information on the forces between atoms, or interactions between magnetic moments. Taipan has been designed to maximise the number of neutrons that reach the sample.

The triple-axis spectrometer is a perfect tool developed for the study of collective motions of atoms in solids. *Double-axis* spectrometers, whether of neutrons or X-rays, consist of a monochromator crystal, the sample and a detector. There are two rotation axes, the first at the monochromator and the second at the sample. In the *triple-axis* spectrometer, a third axis consisting of a crystal 'analyser' is added after the sample. This allows measurement of the neutron energy after scattering, which may in general be different from the incident energy provided by the monochromator. If the incident and scattered neutron energies are equal, there is no net energy transfer to the sample and this is called *elastic* scattering. Elastic scattering typically dominates the scattering from solids, and generally it is assumed in most scattering experiments that the scattering is elastic. If the incident and final energies are different, there is a net transfer of energy to or from the sample and this is called *inelastic* scattering. In solids, the transferred energy is in the form of quantised sound waves or *phonons* (by analogy to photons as quantised light), or *magnons* (quantised magnetic waves) or even as energy transferred to individual electrons, as they jump from one quantum level to another. Typically, the inelastic scattering has an intensity one millionth of the equivalent elastic scattering from a solid.

Double-axis spectrometers measure the total scattering from the sample, assume it to be elastic, and interpret it in terms of the *structure* of the material, while triple-axis spectrometers measure the energy spectrum of the solid, and interpret it in terms of *dynamics* or *how the atoms move*. This in turn tells us about the forces between atoms, or between magnetic moments. This is particularly important in understanding how materials change structure (phase transitions), and in understanding other thermodynamic properties of solids (specific heat, magnetic susceptibility, bulk modulus, etc.).

Triple-axis spectrometers provide *spectroscopic* information with much more detail than than obtained from optical spectroscopy methods like infra-red or Raman spectroscopy. The difference is that, in addition to thermal neutrons having wavelengths comparable with comparable with interatomic spacings, they also have energies comparable to vibrational energies in solids and *inelastic neutron scattering* provides additional information on the spatial nature of the modes or excitations.

Applications

TAIPAN is ideal for the study of phonons and magnons in materials, and in studying the physics of phase transitions and processes where thermal energy are involved. These include strong magnets, superconductors and strange metallic states.

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[Taipan home page](#)

2900 The X-Ray Reflectometer

Description

The X-ray reflectometer is a Panalytical X'Pert Pro instrument. The instrument is capable of measuring reflectivity at air-solid or air-liquid interfaces. The X-ray reflectometry method provides information complementary to that from neutron reflectometry which is available at OPAL. The X-ray reflectometer is used for research on thin-films and surfaces by the Australian scientific and industrial communities. The sample geometry is horizontal with (specular reflectivity) taking place in the vertical plane. It is suitable for the study of air-solid and air-liquid interfaces (i.e. horizontal surfaces).

The X-ray reflectometer is equipped with a Cu tube source with parallel beam optics, motorised beam defining slits, an automatic beam attenuator, a "De Wolf" beam knife and a Xe scintillator detector (capable of >106cps). Solid samples will be mounted on a motorised XYZ, Phi sample stage while a motorised Huber stage will be employed for liquid studies.

Applications

X-ray reflectometry is used to probe the structure of surfaces, thin-films or buried interfaces as well as processes occurring at surfaces and interfaces such as adsorption, adhesion and interdiffusion. In particular, recent years have seen an explosion of interest in the biosciences as well as the emerging field of nanotechnology. Applications cover photosensitive films, electrochemical and catalytic interfaces, surfactant layers, polymer coatings and biological membranes. The increasing importance of hybrid materials, the properties of which are determined by their interfaces and the rapid development in the field of thin film technology provides a strong demand for x-ray reflectometry.

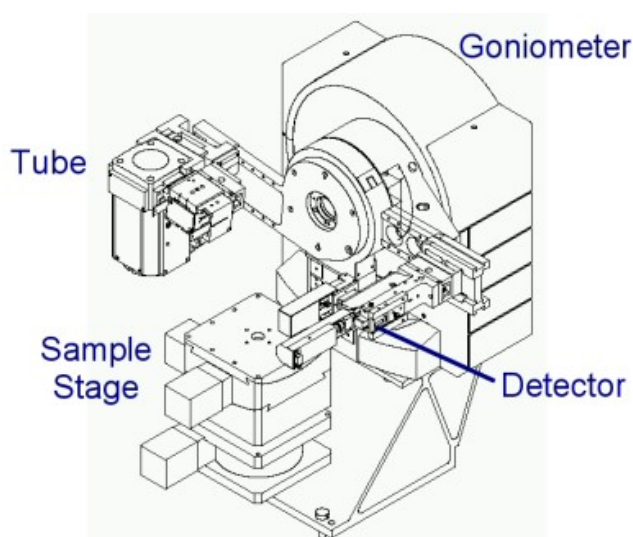


Figure 1. Schematic of the X-ray Reflectometer

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