Australian Government

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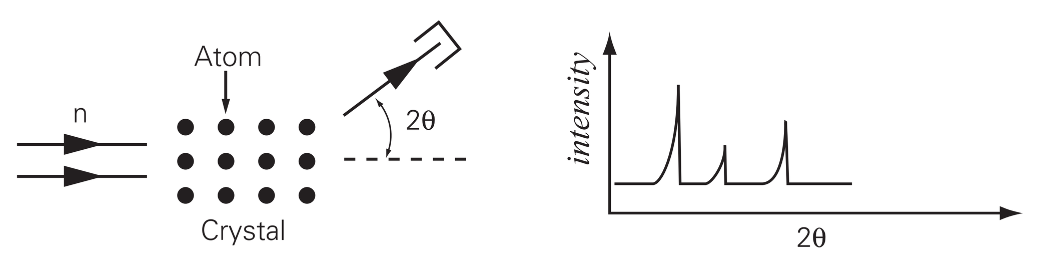
ECHIDNA

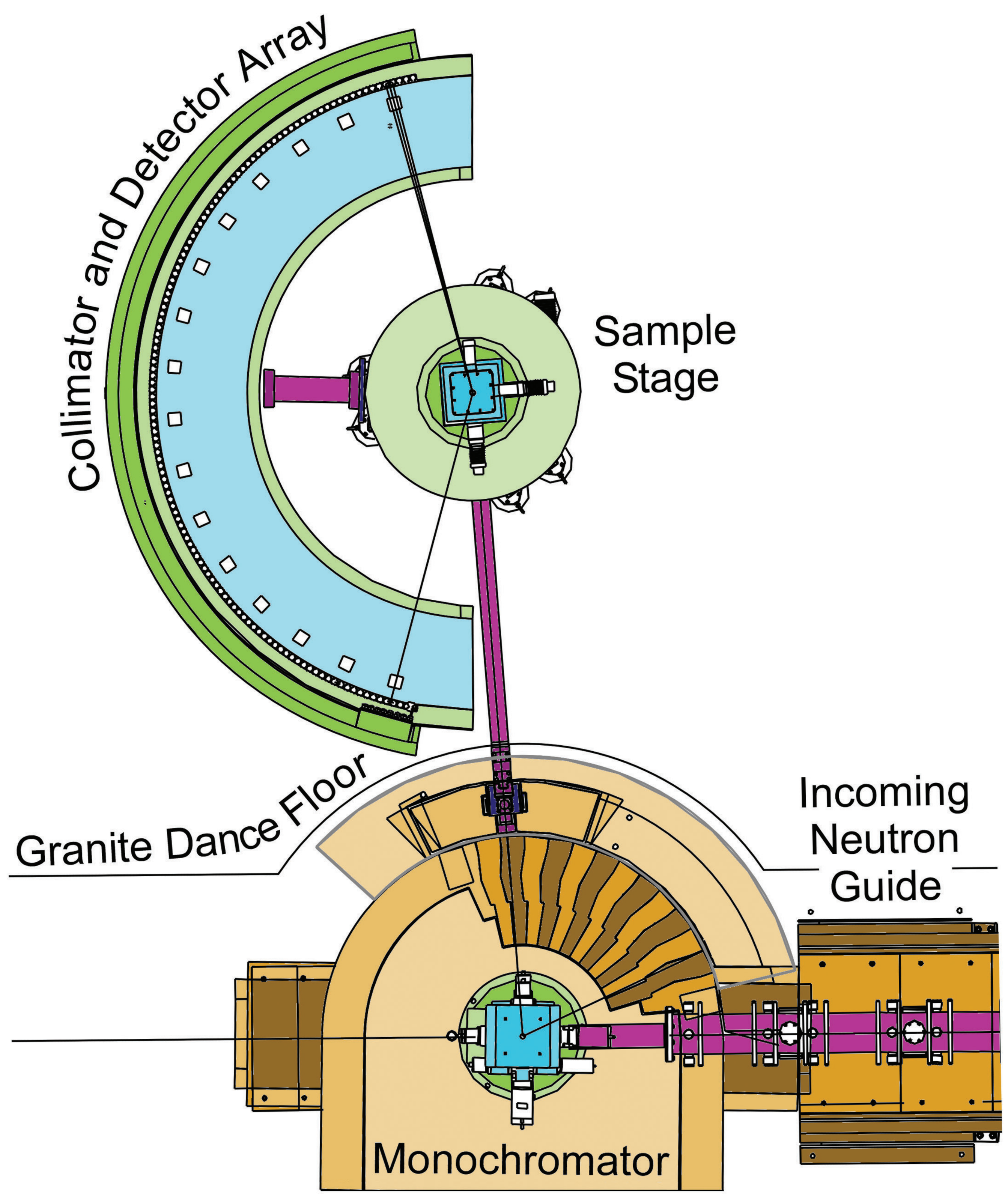
High-resolution powder diffractometer



Diffraction

A neutron beam is scattered within a crystalline material creating diffraction patterns to determine the arrangement of atoms and molecules within the material.

Echidna will be one of the world's best reactor-based high-resolution powder diffraction instrument. Structures that have been determined by powder diffraction include superconductors, pharmaceuticals, aerospace alloys, cements, minerals, zeolites, hydrogen storage media, and optical materials.



What makes Echidna special?

Echidna uses a single wavelength and a highly collimated (non-divergent) beam of neutrons to improve resolution. The high-resolution enables closely-placed peaks in the diffraction pattern to be separated. This diffraction technique can resolve structures very accurately to provide precise atomic and magnetic structures of the sample.

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 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.

Instrument specifications:

Echidna is located on the thermal neutron guide TG1

Wavelength range: 1 – 3 Å (6.3 – 2.1 $Å^{-1}$)

Range of momentum transfer: 0.35 – 12.5 $Å^{-1}$

Max. beam size: 20mm wide by 50mm high

Flux at sample position: up to 10^7 $ncm^{-2}s^{-1}$

Monochromators:

- Ge 115 monochromator, sagittal focussing with fixed radius - 24 crystal slabs
- Ge 335 monochromator, [-1 1 0] vertical allowing for asymmetric reflections, variable sagittal focussing

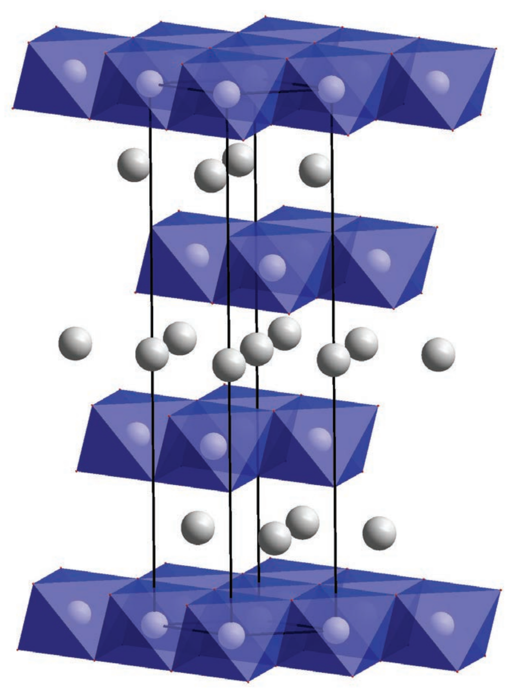
Detector:

- Typical scan time: 2-3 hours
- 128 position sensitive detectors of 25 mm diameter x 300 mm high (active length), 10 bar (charge division)
- 128 collimators with 5' collimation, 15 mm x 300 mm (W x H)

Case Study 1:

Studying cement – making better building products

Using Echidna, cement manufacturers can take the guess work out of which additives to use and how to process them to engineer stronger cements. As the world's most popular building material it may seem surprising that the main component responsible for cement's strength is not completely understood structurally. This material, tricalcium silicate, has a very complicated crystal structure and exists in several different crystal forms known as polymorphs. Each polymorph can be stabilised in cement and has different strength properties and using a neutron diffraction instrument such as Echidna, is the only way to quantitatively determine these forms in cement.



One of the modifications of lithium cobaltate, $LiCoO_2$, a very popular battery material.

Case Study 2:

Lithium batteries – increasing their life

Neutron diffraction is the only technique that can be used for studying real products in real life conditions. With neutrons, we can study a real battery instead of a model electrochemical cell and follow phase transformations in electrodes as a function of charge/discharge cycling or time under load.

With Echidna we can study:

- phase composition of electrodes and weight fractions of phases
- crystal structural characteristics
- particle size and microstrain

This reveals what is happening within the battery during the charging/recharging cycle and is essential for understanding mechanisms of capacity fade and performance optimisation (capacity, charge/recharge life).

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