MANCHESTER
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X-RAY DIFFRACTION CAPABILITY

Overview
X-rays can be used to probe the repeating array of atoms that make up crystal structures; this is done through x-ray diffraction (XRD). This technique gives us information not only about the geometry and size of this repeating structure but also of its quality, orientation and thickness of the films that we are probing. Being a non-destructive technique, it can be used on the most precious of samples with high level of reproducibility.

When looking at thin films, the relative structure of both thin film and underlying material becomes important, with crystal structures of underlying materials sometimes dictating the geometric qualities of subsequent films. The impact of changing these parameters can manifest itself in many ways from changes in chemical reactivity to electrical conductivity.

Thin films characterisation can prove to be problematic when looking at films under 5nm thick, but the sensitivity of XRD gives the researcher capabilities to do so. XRD can also be used not only for single-layer but multiple-layer analysis, observing these parameters for all layers simultaneously.

Capability profile
System: Rigaku SmartLab XRD

X-ray diffractometers suitable for investigating structures of nm-thin films.
The XRD system will allow us to investigate the in-plane and out-of-plane crystalline structures of thin films, laminates and membranes (eg. graphene or graphene oxide membranes) at various conditions such as different temperatures and different solution or solvent environment.

The understanding of the membrane structure at various conditions is crucial for the optimisation of membrane design for various applications. For example, the inter-layer structure of graphene oxide membrane changes drastically with exposure to different aqueous solutions and this property allow us to tune the graphene capillaries in the graphene oxide membranes.

This XRD machine will be critical for the characterisation and functionalisation of solution-processed, large-area, 2DM van der Waals heterostructures and films for various applications such as photovoltaic, sensors etc, which are in the focus of the work at Manchester.

X-Ray tube power 3kW (optimised to measure thin films [eg. 2nm to 10μm])

Incident optics (supporting parallel beam, Bragg-Brentano, mono-chromator, range of slits (inc. Soller), pinhole configuration

Goniometer, range of scanning modes (ϴ - 2ϴ, rocking curves, Omega 2-Theta, grazing incidence, X-Ray reflectivity

Stage resolution < 10mdeg

Step size accuracy < 0.1mdeg

Goniometer range (minimum) (-5 to +85 Deg)

Degrees of freedom to include z, phi, chi (or equivalents)

Detection optics, (range of slits, inc. Soller)

1D detector with high dynamic range

0D detector

In plane measurement capability

Holding standard samples up to 50mm diameter

Automated sample/X-ray alignment

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Z sample movement (> 45mm)

Controlled Heating stage >1000°C (inert Atmosphere)

Temperature control stage (-100°C to 350°C) (inert Atmosphere/Vacuum)

Ability to measure air sensitive samples (>2 hours measurement time)

Cabinet space to accommodate additional measurement equipment (eg. 2 x Keithley 2400 source-meter or similar)

Cabinet to provide additional AC power outlets for measurement equipment (DVM) and lead through capabilities; BNC connectors, USB etc