

Microdiffractometer MD2*



Leading edge technology for high quality data collection

- ◆ Full remote control
- ◆ Low background
- ◆ Air Bearing Goniometer
- ◆ Unrivalled sample and beam viewing

Designed for high throughput

- ◆ Automatic sample alignment
- ◆ Sample changer compatible
- ◆ Automated beamline compatible

Unparalleled user friendliness

- ◆ Full remote control
- ◆ Convenient Graphical user interface
- ◆ Built in tuning and diagnostic tools

Fully integrated

- ◆ Provided with computer and control software
- ◆ TANGO device server for remote control

The **Microdiffractometer MD2** is designed to perform the most demanding X-ray macromolecular crystallography experiments and offers a control interface suitable to automated beamlines.

Once a sample is mounted on the transfer arc, users can control the processing of the sample without the need of entering in the experimental hutch. Operations like beam locating, crystal centring and crystal alignment are performed from a graphical user interface. As well, the **Microdiffractometer MD2** can be fully controlled by a host program through a CORBA device server.

Concept: the integrated beam collimation devices define the beam of a desired size and minimise air scatter. The video-microscope looks in the direction of the beam and monitors the beam and the sample position without parallax error. The beam or the sample can be observed remotely, at any time.

Benefits: a precise part of even a small crystal can be irradiated with a minimum background. This is of prime importance to get high quality data from micro crystals, weakly diffracting or mosaic crystals. The full remote control accelerates standard experiments, giving to the users an unmatched ease of use. Samples as small as 10µm can be aligned with a 10µm beam in few mouse clicks.

Highlights:

- ◆ Integrated beam shaping: 5 to 100 µm beam - air scattering shielding and beamstop.
- ◆ Fast & High precision PHI axis: 2 µm SOC radius; down to ±1mDeg RMS error @10 Deg/s
- ◆ Optional MiniKappa goniometer head (optional)
- ◆ Optional assisted sample transfer with motorised arc
- ◆ Compatible with the EMBL sample changer
- ◆ Assisted (3 clicks on sample method) or automatic sample centring and alignment
- ◆ Beam viewing*** and sample viewing with a parallax free video-microscope***
- ◆ Optional fluorescence detector (for MAD experiments)
- ◆ User friendly GUI
- ◆ Integrated tuning and diagnostic tools
- ◆ Full remote control

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Description* and main specifications*


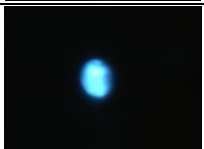

PHI axis

Single horizontal air bearing axis, driven by a torque motor (no gearbox), coupled to a motorised sample-centring table and mounted on a motorised XYZ table.

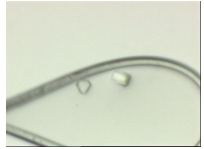
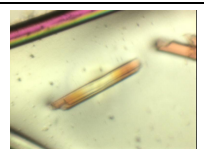
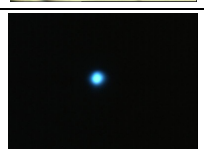
- ◆ Free rotation
- ◆ Max rotation speed 120Deg/s
- ◆ Positioning error ± 2 mDeg (HP option ± 1 mDeg)
- ◆ Following error $< \pm 1$ mDeg RMS@ 10 Deg/s
- ◆ $2 \mu\text{m}$ sphere of confusion radius (sample off centring $< \pm 1$ mm)
- ◆ Sample centring range ± 2.5 mm;
- ◆ Sample length adjustment (Y) ± 6 mm.
- ◆ Fast multi pass.
- ◆ Minimum sample to X-ray detector distance 60 mm

Diagnostic tool: rotation speed precision (Following error plot)

Beam shaping (Pictures MD1 – ESRF ID13)

	No shaping	Beam definition/cleaning aperture Available in 5 to 100 μm size, collimates the incident beam to the desired size: easily replaceable, mounted on supports at about 20mm from the sample on a motorised YZ table. The use of the definition aperture is optional when the beam is defined forward by slits. <i>Tuning tool:</i> alignment procedure using the internal beam photodiode (YZ scans).
	100 μm cleaning aperture	Beam cleaning aperture and beamstop device Reduce air scattering, cuts the beam definition aperture scatter and protects the detector from the direct beam. Composed of a 100 to 200 μm aperture mounted at the end of a beam shielding capillary plus a beamstop. <i>Tuning tool:</i> alignment procedure using the internal beam photodiode (YZ scans).
	30 μm definition aperture + 100 μm cleaning aperture	Beam cleaning aperture and beamstop device Reduce air scattering, cuts the beam definition aperture scatter and protects the detector from the direct beam. Composed of a 100 to 200 μm aperture mounted at the end of a beam shielding capillary plus a beamstop. <i>Tuning tool:</i> alignment procedure using the internal beam photodiode (YZ scans).

Video-microscope (Pictures MD1 – ESRF ID13)

	10 μm sample	Camera Sight coaxial to the beam to see the sample or the beam (scintillator) without parallax error: High resolution (0.28 N.A. objective lens); 12X motorised zoom; 576 x 768 pixels display; condenser lighting with polarizer and motorised analyser. Field: About 1.8x1.5 mm @ zoom min, 0.18x0.12 mm @ zoom max.
	12 μm needle (zoom 10)	Beam viewing scintillator Fluorescent single crystal mounted on a motorised support. Allows to control the beam shape and position; exploits the full video-microscope resolution; can be set remotely at any time, even when a sample is mounted on the PHI axis (sample is shifted); set in the sample plane to visualise the beam exactly as hits the sample (with the aperture and beam cleaning aperture set).
	30 μm beam (zoom 6)	

Sample changer compatibility

The MD2 is compatible with different sample changers through a compatibility kit (See options)

Beam intensity measurement photodiode

Pin photodiode mounted below the beam viewing scintillator and connected to a programmable gain amplifier: Used for tuning the shutter delay, aligning the apertures and monitoring the beam intensity.

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(Not for on line beam monitoring). Can be set remotely at any time, even when a sample is mounted on the PHI axis.

Shutter command generation

Precise TTL output generated by hardware comparators connected to the PHI axis encoder register: Shutter open and close delay compensation.

Tuning and diagnostic tools: plot of the command output or beam intensity versus the PHI axis angle (using the internal beam photodiode); automatic open and close shutter delay calculation.

Miscellaneous

Compatible with the OXFORD CRYO SYSTEMS™ cryo-cooler (not included)

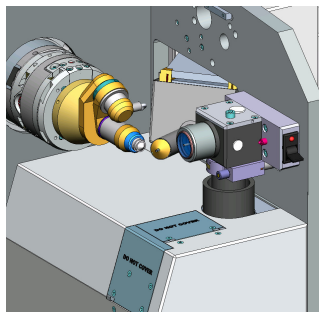
Overall dimensions: 280 mm (width without options) x 490 mm (depth without connectors) x 520 mm (height). Weight: about 140 Kg; Beam to support table height: 410 mm minimum

Power: 220V50Hz 10A

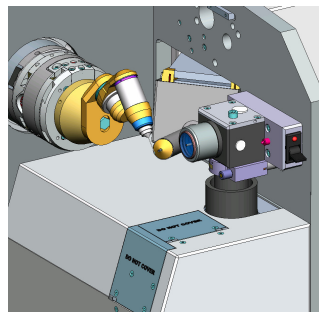
Air supply: 6 Bars compressed air (Oil free, Filtered <10µm) and 10.5 to 12 Bars compressed air @<60 standard litre/minute (Relative humidity <85%, Oil free, Filtered <5µm)

Options

- ◆ HP Grade PHI axis encoder: Positioning error < ±1 mDeg.
- ◆ Fluorescence detector translation table compatible with Roentec XFlash 1000x (Tube length 100). Others detectors on request.
- ◆ C3D Automatic loop centring software, C3D Automatic crystal centring software
- ◆ Sample changer compatibility kit with a sample changer using SPINE type Sample Holders. The kit is composed of Hardware, electronics and software.
- ◆ Kappa Head. Allows remote orientation of the sample (Data collection with 0 to 48 Deg. tilt). Replaces the Sample transfer Arc (when set at 48 Deg). Designed for SPINE sample holder length. Compatible with the SC3 Sample Changer. Not compatible with the Motorised sample transfer arc.



Tilt = 0



Tilt = 48 Deg

- ◆ Motorised sample transfer arc: Assists manual mounting of pre-frozen samples (stored in HAMPTON magnetic CrystalCap™/vial sample holders); cryo-back switch to facilitate sample mounting; automatic transfer to PHI after the sample holder is placed on the arc. Not compatible with the Motorised Kappa Head.

Control electronics

It consists of an electronic rack installed close to the **Microdiffractometer MD2** (at up to 7 meters). The rack is connected to a Windows XP PC via a private Ethernet link.

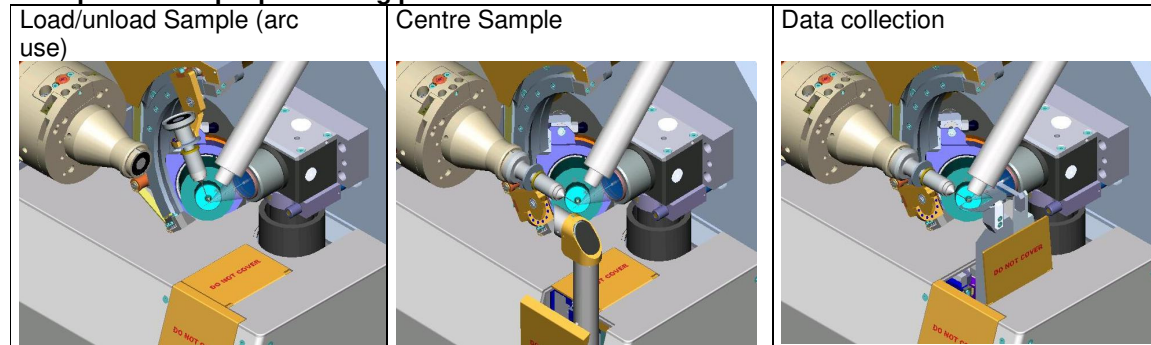
Control software

The **Microdiffractometer MD2** is controlled from the PC through a GUI or by a host program through a CORBA device server. The main GUI window is divided in three areas. The first displays a view of the **MD2**, the second displays the video-microscope images, and the third area is for controlling the processing of the samples.

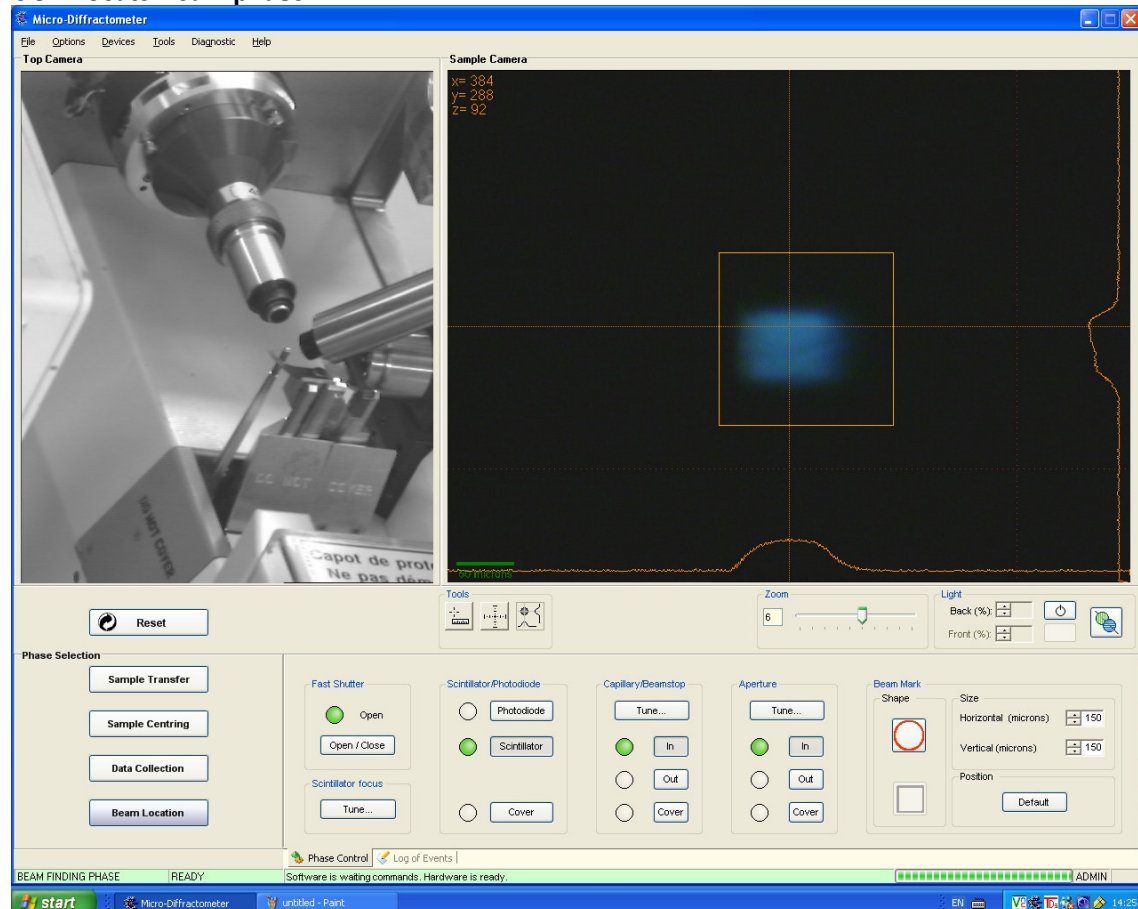
Operations are managed through six phases: "Load Sample", "Centre Sample", "Locate Beam", "Align Sample", "Data collection" and "Unload Sample". Once a phase is selected, the useful controls are visible on a control pane.

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Examples of sample processing phases

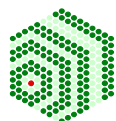


GUI: Locate Beam phase



View of the beam using the scintillator – Courtesy of ESRF ID14-3

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