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High-precision multipurpose diffractometer

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Abstract
Here we present the results of re-developing of a Diffractometer (Dm) derived from an upgraded process in a synchrotron beam line (ID10B/ESRF). Our efforts were successful in achieving the required high-precision by adopting the maximum the accumulated expertise and advanced knowledge in precision field inside of a 'design for costs' concept. The new machine is built on a previously standard - four circles Diffractometer (Dm4) and a Double Cristal Deflector (DCD), now working together and performing, vertical and horizontal advanced scattering investigations. New high precision positioning (Rd_Tripod/PKM) and metrological (LION) devices have been conceived to be used and comply with the micro/nano parameters of accuracy, e.g. SoC (Sphere of Confusion). This approach can be used to guide similar future projects.

Synchrotron Machine Design, Manipulation, Positioning, Precision Measurements, X-ray

1. Introduction

Probing matter at the micro and/or nano level is an active topic of research - and, the synchrotron X-ray is a proven powerful tool for such investigations. Based on precision diffraction techniques (Df), the physical/ chemical properties of various materials are collected by dedicated machines (e.g. diffractometers) and then analysed and interpreted. However, is aneed for improved precision in such approaches; meaning that either new equipment must be developed or the current devices significantly improved. TROIKA II (ESRF/ID10B) was conceived as a versatile beamline for the study of liquid/solid interfaces using high resolution X-ray scattering/diffraction techniques targeting the 100-1000 nm range [1]. By combining multiple techniques e.g. GID, XRR, SAGIXS into a single instrument, both horizontal and/or vertical scattering methods were possible to be applied. Untill now, in the Experiment Hutch (EH), two separated systems– the diffractometer (Dm) and deflector (Df) worked together. However, by following an upgraded process, the structure of the beamline has been modified [2] to increase the performances. It is necessary that the Dm and a double crystal deflector (DCD) work together in a more precise manner within the same limited space available – and together with several environmental instruments (e.g. the Langmuir or Bragg). In addition, all of the components that could potentially be recovered from the currently used devices should be reused (to be cost effective).

2. Working principle

The working principle for the new/improved Dm&Df equipment with the most important motion parameters are shown in Figure 1 and Table 1. The entire concept is built around the powerful 2+2 scattering geometry of a Dm (Dm4), providing a compact motion axis arrangement. Horizontal and/or vertical scatterings are possible by the co-relative motions of the detector (D) - C_1 & C_2 and samples (S)–C_3 & C_4 around the centre of rotation (C) and the incoming beam (X_i) performed with high precision, as derived from diffraction physics and the techniques applied.

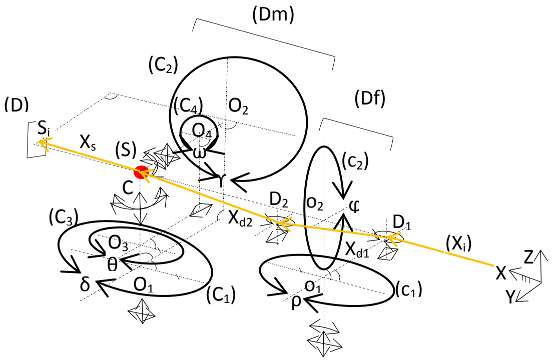

Figure 1. Dm (&Df) – Basic working principle

The deflector optical device (Df) is deflecting the incident beam (X_i) with small angles (1-8°), especially in the horizontal scattering case, by using two special mirrors that are positioned relative to each other with high precision. This is based on a goniometer-(c1)&(c2) Euler cradle (E) motion principle. The correlated data of diffracted/scattered points (S_i) and the motion axis position parameters ($\Upsilon\delta\omega\theta/\varphi\rho$) are finally collected and analysed, including: X_i,X_d,X_s - incident /deflected / scattered X ray; (C_i), i=1-4-Motion Circles; $\Upsilon\delta\omega\theta/\varphi\rho$-Angles; C - Centre of rotation; D_i; i=1,2-Deflection points; XYZ-Reference system; R/T - Rot./Trans., Rep-Repeatability and MIM-Minimum Incremental Motion.

Table 1 Dm & Df – Motion parameters

Component		Parameter (leng/ang)	Range [mm/deg]	Rep./MIM [µm/µrad]	Note
Dm	D	C1(δ)-Rz_D	135/-40	0.6/1.7	ϒ=90°
		C2(ϒ)-Ry_D	15/-195		δ=0°
	S	C3(θ)-Rz_S	±180		Tx=-0.5m
		C4(ω)-Ry_S	±180		
Df	E	c1(ρ)-Rx_E	±130	1/0.9	
		c2(φ)-Rz_E	±180	35/0.9	Wobble=1

3. Design concept

The entire Dm (& Df) working principle can be seen as an inter-correlated motion of several high-precision positioning manipulators (PM) for: a) Detector (D); b) Sample (S); and c) Light (Xray), Fig.2. Each of them designed using preponderantly high-precision rotations (or gonio/G) positioning units (Pu) [3]. The Detector arm (Da) PM is solely responsible for: a) horizontal; and b) vertical circular motions carrying various detectors' set-ups (max. 1.5m/40 kg) in both scattering geometries (H/V) and is based on the perpendicular arrangements of the two gonio (G480). The sample positioning (S) PM provides a flexible means for positioning the sample together with bulky environmental instruments (e.g.390×590×500 mm/150kg/- H or ϕ200mm/10kg - V) and consist of: a) gonio (G420/reused & G410); b) circles segments (χφ/5203&5204); and translations (Z/ 5103 & XY/5102) units.

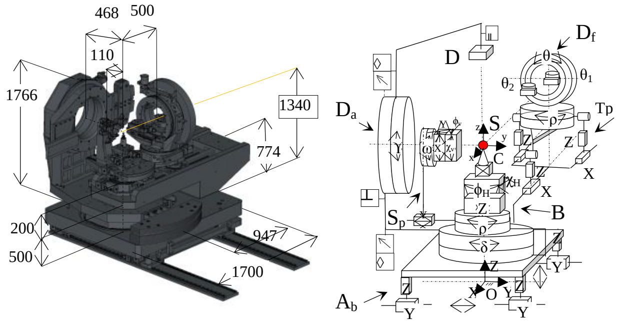

Figure 2. Dm (&Df): L–3D and R-kinematics views design

The X-ray PM is responsible for directing the X_i beam towards the sample comprising an Euler cradle with two gonio (G440 &G430/reused) units supported by a new high precision 2dof Tripod(Tp/Z=±10mm/10µm;Ry=±5mrad/5µrad) with redundant (Rd) parallel kinematics mechanism (PKM) [4] using three Z/ 5103 [3] stages. In addition, two separated Pu (G410) have been used for manipulating the mirrors to deflect the beam. The Df can be moved along three sliding guides (Y=1m/10µm) located on a strong granite bridge (B) - fixed at one end and adjusted by screws at other one. A PKM Alignment base (Ab) with 1dof (Z=45mm/10µm) supports and move all in vertical direction. (Note: The values are representing the stroke/MIM).

4. Prototype

A manufactured product has been realized based on the above design considerations. Despite the fact that this was built using high-precision components (e.g G/X3 class) and high-precision assembly procedures, most the performance parameters have been further improved and several mounting/demounting and trial/test procedures applied.

5. Accuracy

Accuracy of motion is a permanent concern in positioning industry; especially for Diffractometers implying an appreciable number of motion axes (Dm&Df =33) and loads (150kg). As for every serial (stacked) manipulator, each axis is prone to errors; and, it is coming in the total error budget with a part (except perhaps the PKMs). However, for most of the working configurations the Dm&Df is extensively using only some of motion axes performing the detector (D) and sample(S) circular (and, spherical) motions around the C (CoR). In order to minimize the errors, an identification &acting process has been initiated at: a)the individual(Pu); and b)the (sub) assemblies' levels. The real/on-site results have been compared with the existent ones from the accuracy protocols. Following this, several types of errors: a) standard (wobble, run out) and b) geometrical (planarity, perpendicularity) were constantly minimized. Even the design concept was slightly re-evaluated for additional solutions (adjusting screws (B)). The standard precision instruments (e.g. laser interferometers, electronic length measurements) and dedicated measuring devices had been used. In the case of Sphere of Confusion (SoC) error determination, the usual metrological device consisting from a supporting bar (Al) with a digital dial gage (TT60/TESA/1µm) at one end has been reconsidered as the measured values approached the limit between micro & nano. It proved to be itself prone to errors. In the horizontal position, the deformation by 200 g (dial gage & support) was 15µm, Fig.3. (A FEA model confirmed the finding).

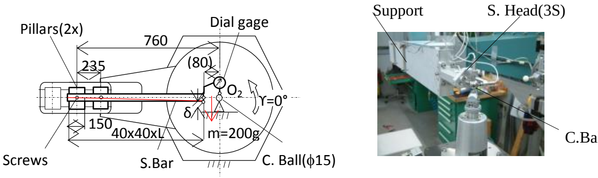

Figure 3. Measurements: L-standard (touch) and R-new (capacitive)

A new measurement device has been produced by re-designing (stiffer) the support bar and for greater sensitivity nanometres inspection device(CPL290/LION/1nm)[5] implemented.

6. Conclusions

SoC is the principal parameter for Dm accuracy evaluation. SoC maps the error resulting from the relative motion of main components (Da and Sp) around the virtual CoR(C). The obtained values from sequential (angular steps) in full/partial circular motions are registered for all sensors (S_i, i=1,2,3) as polar diagrams. The max diameter (d_M) of a virtual sphere enveloping the max values (d_i, i=1,2,3) expresses the SoC; for standard machines it is usually between 50-100 µm [6].

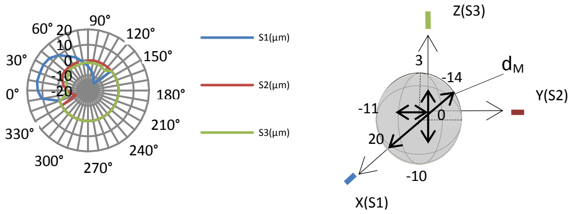

Figure 4. SoC (Da): L-Polar diagrams and R-Spatial representation

By improvments and the use of a new 3D measuring tool, results are being generated more directly (and precisely), Fig.4.

Table 2 SoC Numerical Values

Accuracy	Component	d_M(µm)
SoC	Da	34
	Sp	5

The maximum obtained value for Da (34µm) is the best in Dm4 class, Tab.2. And, the work behind, a prove of pushing the actual existent limits of the accuracy for such machines.

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