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POLAR SYNCROTRON DIFFRACTOMETER

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Abstract

A new product for research purposes aiming to work in a 4th generation synchrotron facility (APS-U) after its upgradation has been recently developed. POLAR-Dm was conceived on a traditional 6C (C-circles) geometry, maintaining the common kinematic structural principle of the family. With the addition of several interchangeable devices, the multipurpose system is expanding the spectrum of possible investigations, maintaining the precision of setups. Mainly, it consists of two customized sample (S) modules for high-precision versatile sample manipulation and a dovetail detector arm (D) module for manipulating the detector, optics (polar analyzer), slits, etc. An alignment base (Ab) module stable supports the above modules and roughly adjusts the motions towards the incoming X-ray beam. In addition, a planar non actuated manipulator is facilitating the cable management during the work. The kinematic, design and precision concepts applied, together with the obtained test results are all in detail presented.

INTRODUCTION

The advanced synchrotron investigations require not only improved beam characteristics and/or new modern techniques, but dedicated instruments adapted to the specificity of the applications.

Advanced Photon Source (APS) research facility is currently under an upgradation process (APS-U) [1]. Apart from several improved characteristics e.g., emittance, coherence, etc for new / enhanced beam lines, an appreciable number of experimental stations (hutches) are to be developed and/or improved, as well. Several beamlines will be allocated to magnetic materials (MM) group from X-ray Science Division (XRS). After its completion, the 4-ID (POLAR) beam line will investigate the emergent electronic properties (e.g., inhomogeneity) of advanced magnetic and ferroelectric functional materials, relevant to quantum and energy technologies, using spectroscopy and/or X-ray magnetic scattering techniques [2].

A request to develop a dedicated diffractometer has been issued for one of the end stations (G) [3]. The intention was to use a common fife-circle (5C) diffractometer architecture adapted with the geometry for horizontal scattering (Q-range access) for a superconducting magnet (2T) and low vibration for thin films, under extreme conditions - low temperature (cryo) and high pressure (HV) investigations. In addition, adequate support for a vacuum polarizer analyzer and area detector has to be included. The new Dm has to offer not only heavy load/small manipulation capabilities, but (high) precision features, as well [4].

The main features of the final product (prototype) are described below, including most important aspects related to kinematics, design and precision concepts.

POLAR DM

Dm should accommodate with the use of x-ray techniques based on spectroscopic (absorption, polarized dependent resonant) and magnetic (XRMS) scattering principles. A 2T magnet sample (120 kg), sample cells (30 kg) and (15 kg), together with small (200 g) one must be manipulated by the two sample positioning systems. 1D/point (5 kg) detector and the polarized analyzing optics (100 kg) are to be manipulated, as well. The manipulation errors must be inside of the Sphere of Confusion (SoC < 50µm).

Kinematics

Basically, from a kinematic point of view, the chosen Dm (POLAR) architecture belongs to 5C (2D + 3S) class – two (C_i, i = 1,2) for detector(D) and three (C_i, i = 3…5) for the sample (S) actuated circles, respectively [5]. However, as (S) comes with two independent setups called manipulators (S_1, S_2), each of them is composed from another actuated circle $(C_6)_i$, i = 1...2. Thus, the structure became a 6C (2D + 4S). However, there are also another three (3) circles inside of the polar analyzer (C_7 - C_9), so the entire system falls into a multi-circles Dm class.

Mainly, it has two distinct (kinematics) chains (K_D, K_S) supported by another (K_B), Fig. 1. The experimental investigations are based on the corelated motions (positioning) of the two (K_D, K_S) relative to X-ray (incident/scattered) fixed beam, respecting the diffraction law (Bragg).

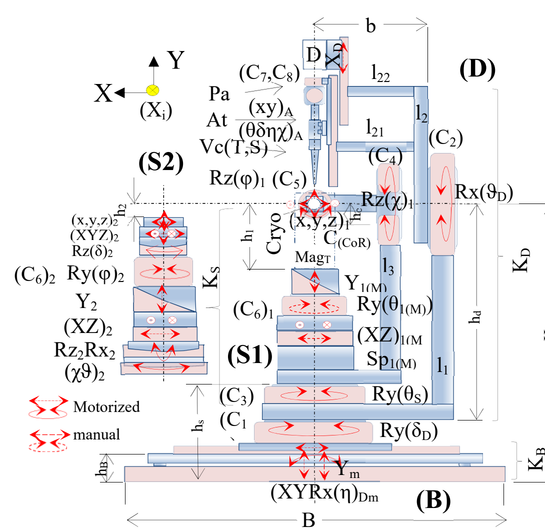

Figure 1: POLAR-Dm kinematics.

The detector (D) manipulator kinematic chain (K_D) mechanism consists of two active rotational joints C_1 (δ_D) and C_2 (ϑ_D) linked together through (l_1). In addition, a dove

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tail arm (l_2) supports two linear sliding guides (L_{21}, L_{22}) to accommodate with the use of different detectors and polar analyzer (An) instrument, catching the scattered X-rays. In addition, the polar analyzer mechanism is based on a combination of three orthogonal motions C_7 ($\theta_X = \pm5°$) / C_8 ($\delta_X = \pm10°$), C_9 ($\eta_Z = +30° - 110°$) and C_{10} ($\chi_Y = \pm5°$).

The sample manipulator (S) is composed of two configurations (S1, S2) corresponding to two distinct serial kinematic chain (Ks = 1,2) mechanisms.

In its first configuration (S1) two orthogonal circles C_4 (θ_M) and C_5 (χ) supported by C_3 (θ_S) are forming an opened Euler cradle mechanism ($\chi = \pm100°$), holding an instrument (cryostat) to move in (XZ = ±2 mm, Y = ±3 mm). The access to the sample (setup, maintenance) is almost entirely free, opening the way for large (and, heavy) load sample manipulations (magnet). In addition, on a strong support (Sp) translational & rotational (manually) driven devices $(X, Y, Z, \theta)_M$ are included. Note: The cryostat tip performs spherical motions around the fixed point (C), called center of rotation (CoR).

In the second configuration (S2), the kinematics consists of several precision positioning devices which are stacked one on the another starting with two (2)-partial rotations $(\chi\vartheta)_2$, following a displacement for all three axis $(XYZ)_2$. On top of them, a high precision device performing full–$Ry(\varphi)_2$ / $(C_6)_2$ and partial - $Rz(\delta)_2$ rotations are carrying a course $(XYZ)_2$ and precision translational devices $(xyz)_2$.

Note: C_3 is a common actuated joint (circle) for both configurations (S1, S2).

An alignment base (B) has to support the above structures, providing stiff and short motions - Y, X = ± 20 mm and $Rx(\eta_{Dm}) = \pm5°$ for roughly alignment against X-ray. The main Dm motions, together with their range and precision parameters are included in Table 1.

Table 1: POLAR-Dm Basic Motion Parameters

Circles 5C (6C)	Range (°)	Rep.* (″/ µm)	Res.* (″/ µm)	SoC* (µm)
C_1	($\delta_D = \pm180$)	8	3.6	15
C_2	ϑ_D = -30+180	0.5	3.6	15
C_3	$\theta_S = \pm180$	0.5	0.36	0.1
C_4	$(\chi_S)_1 = \pm100$	8		5
C_5	$(\varphi_S)_1 = \pm180$	8	3.6	50
$(C_6)_{1/2}$	$(\theta)_1/(\varphi)_2 = \pm180$	8	0.5/3.6	5/15

* At least (<)

An overview of the most important motorized motions performed is shown in a short simulation video [5].

Note: O-XYZ, is a right-handed set of orthogonal axes with Z (+) along the X-ray beam and Y (+) vertically upwards; O ≡ C (CoR).

Design

A modular approach has been applied in the design process [6], adopting the detector, sample and base manipulation subsystems, as main positioning modules (Pm_i, i = 1,2,3), Fig. 2. Each of them built from a (stacked) combination of several linear/rotational Positioning units $(Pu)_i$.

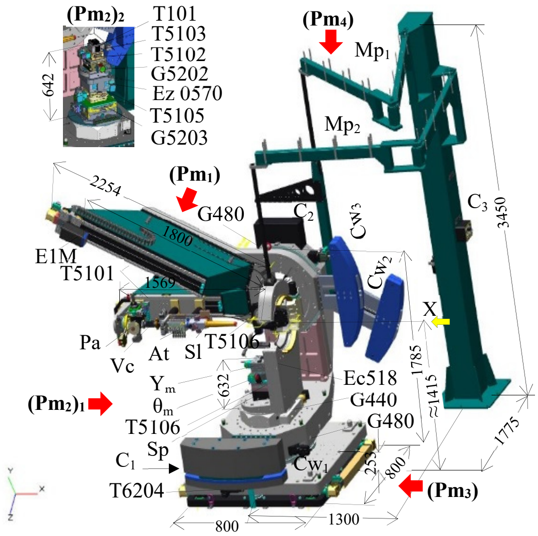

Figure 2: POLAR-Dm CAD layout (3D).

Due to the long arm carrying the necessary detection and auxiliar devices, the detector (D) positioning module (Pm_1) was built (first time) on two similar heavy load precision gonio(s) - G480 with vertical(V) and horizontal(H) axis. They provide the necessary actuation forces (moments) to manipulate: a) detector (Eiger1M/5kg), b) ancillary devices - polar analyzer (Pa/15kg), attenuator (At/3002) and vacuum tube (Vc/12kg) & slit (JJ-Xray/IB-C30-HV) together with their supports (linear stages, etc). The (Pa) has been built on a combination of two gonio - G410A/G409 (XEW2), one linear (T5101/XE) and head (H1005) Pu(s).

Note: Solutions have been applied for the static balance, using counterweight (Cw_i, i = 1…3).

In the first configuration of the sample (S1) the module $(Pm_2)_1$ a dedicated open Euler cradle device (Ec518) based on a combination of two active positioning units (Pu_i, i = 1,2) called Goniometers (Gm) or simply gonio (G) linked together, as described before, is used. The device is completed with a linear translation stage – XYZ (5106/XE), carrying the cryostat (ARS DE-202G/ARS).

Note: The value of reproducibility following the interchanged operation for Ec module must be inside of 50 µm.

In the second configuration (S2) = $(Pm_2)_2$, a high precision goniometer system is built on two gonio segments (G5203/XE), supporting a XYZ translational stage (5105 XE) on which a high speed (and, high precision) air bearing stage (EZ0570) is located. On top of it a (segment) stage (S5202/XE) is supporting a combination of two translational stages (5102&5103/XE) on which the nano positioning(piezo) stage (Tritor101 CAP /JENA) was fixed.

All above Pu(s) for both configurations are moved in rotational motion by a precision gonio (G440/XEW2).

The alignment base (B) module $(Pm)_3$ was designed upon a standard table type (T6204), providing stiff and stabile support (> 1000 kg) for all necessary operations.

An overview of the main features (type and precision) of Pu used is included in Table 2.

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Table 2: POLAR-Dm Basic Motion Axis

Axis	Pu	Prec.	Note
$A_1(\delta_D)$	G480	XEW2V	Pm_1
$A_2(\vartheta_D)$	G480	XEW2H	Pm_1
A_3 (θ_S)	G440	XEW2V	$(Pm_2)_{1,2}$
$A_4(\chi_{S1})/A_5$ (φ_{S1})	G518	-	$(Pm_2)_1$(Ec)
$A_6(\theta)_{1M}/A_6(\varphi)_2$	G409/EZ0570	XEW2/-	$(Pm_2)_{1,2}$

As precision was one of the requirements, *modelling and simulations* using Finite Element Analysis (FEA) have been performed iteratively to estimate the deflections and stresses (von Misses), reducing/eliminating them, e.g., (D), (Ec), slides, etc., improving by this their stiffness. (Ec) being one of the critical components, the specific simulations performed are shown below (Fig. 3).

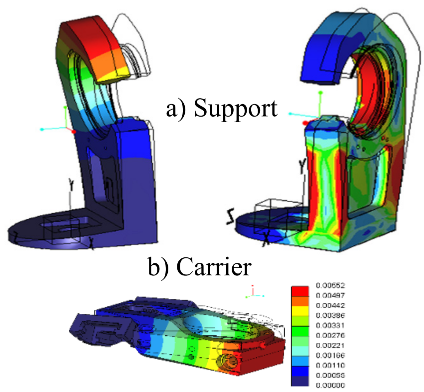

Figure 3: Euler cradle deformation and stresses (FEA).

The control of the actual multi-axis system (Ai, i = 30) has been generally realized, using closed loop – stepping motors (Vexta/ORIENTAL/PK(P)), gears (HUBER) and incremental encoders (Vionics/RENISHAW/RKLC (RES M)). In this respect four power drive (PowerPack) and two driving (SMC9300) boxes have been provided. *Cable management* for a machine with multiple axes is always a challenge. In addition, as in this case, the cables must be directed to the roof electronics, a dedicated module (Pm_4) consisting of two planar manipulators (Mp_1-D, Mp_2-Ec) has been designed. Motor cables are routed to RJ45 jacks and encoders to a DB9 connectors, both at APS-U standard pinned. The connections between wires have been performed through three main (connection) boxes - Cb_i, i = 1…3 (1 = (B) + (S2), 2 = (D) + (Pa) + (At)+(Sl), 3 = Ec). To prevent the crushing hazard, warning stickers have been included, as well. Note: Most of the wires have been chosen to go through (central) holes and/or slip rings.

Prototype

Based on the above design considerations and related documents, the components have been carefully manufactured. The product (prototype) is now in the final step of its assembly, Fig. 4. Attention was given in the machining process for obtaining high quality functional surfaces, respecting the geometrical tolerances, as those in contact with sensitive components e. g., circular/linear guides or measurements bases for instruments. Fine adjustments in the assembly process have been performed mounting the precision components, from the beginning to the end.

After its completion, the prototype will be tested at the factory site from a functional and precision point of view. A factory acceptance test (FAT) report will be issued, before the installation on the indicated premises will be done. All the values of motion and precision required parameters must totally fulfill with the specifications.

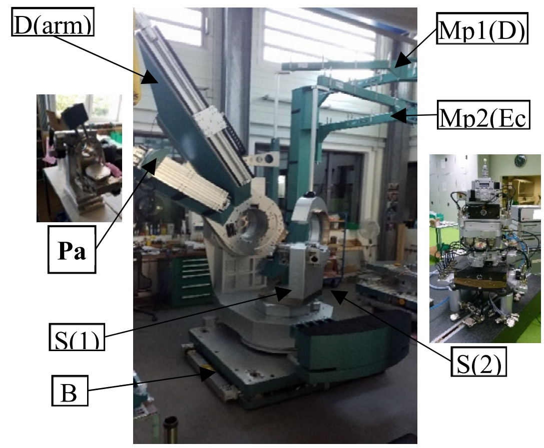

Figure 4: POLAR-Dm Prototype.

CONCLUSION

A new dedicated diffractometer (POLAR-Dm) with flexible capabilities for various X-ray diffraction investigations (XRD) of different magnetic materials able to work in a 4th generation synchrotron facility has been developed. POLAR-Dm has resulted from a successful combination of standard/customized precision components and instruments to use the specific X-ray (magnetic) techniques, under extreme conditions (pressure and temperature), maintaining a high precision manipulation level of both, the heavy and small samples. Mainly, it offers an adequate solution to selective manipulate: a) magnet (2 T) with appreciable load inside of (SoC = 50 µm) and b) smaller loads (30 / 15 / 0.2 kg) inside of (SoC = 15 µm). In this respect, two types of interchangeable devices (Euler, gonio) have been provided with a high rate of reproducibility (< 50 µm). It is expected that due to its specific features, the final product will enhance the investigation capabilities to a new level.

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