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Quantum diffractometers platform

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Abstract
New research instruments for advanced materials investigations, able to explore their quantum properties working in a modern large scale free-electron laser European facility has been recently developed. The project consisted of two dedicated diffraction machines (Dm_1, Dm_2), fully integrated in a common platform (CrQ-Dm) to perform the specific experiments located in the experimental station (Cristallina), belonging to a new beamline branch (ARAMIS3). Dm(s) have been conceived to manipulate heavy loads (<1t) with high precision (SoC<40 µm) being highly compatible between them and others. However, they exhibit notable differences, (CrQ-Dm_1), is dedicated to manipulate the samples under a strong magnetic field (5,2T) and extreme low temperature (<-10mK) and (CrQ-Dm_2), under a pulse (repetition rate 10-30 min) magnetic field (50T) and low temperatures (<4K). In addition, the last one provide means for general use diffraction experiments. Specifically, CrQ-Dm_1 is carrying a heavy load magnet with the adjacent cryo instruments (1t) and CrQ-Dm_2 a smaller load pulse magnet (0.5t). It includes a common body support and alignment table (Tb) on which adequate precision positioning sample stages (Sp_1,Sp_2) and detector towers (Dt_1, Dt_2) will be stacked one after the another, depending of the application specificity. The redundant use of the components increases the compatibility inside/outside of the machines, reducing the preparation time or repairing in the case of unexpected failures. The challenging aspects from kinematic, design and manufacturing points of views, together with the precision achieved for the prototypes are presented.

XFEL, positioning, diffractometers, kinematics, design, manufacturing, precision

1. Introduction

Advanced materials, as Quantum materials (QMs) consists of a special class of materials exhibiting specific properties in the quantum domain [1]. Due to earlier huge, expected potential [2], the research interest became strong [3]. Various applications across diverse domains, as energy, electronics, optics, biology, etc are waiting to use (or, already) used them [4].

However, the uncommon properties e.g. superconductivity, complex magnetism, topological phases, etc comes with additional challenges related with their accurate characterization, through a correct qualitative and quantitative determination of the specific features. The investigations, imply a sophisticated instrumentation, working in extreme conditions, as high magnetic field and low temperature.

X-ray magnetic radiation [5], coming from large scale facilities, as free electron lasers (FEL) proved to be a useful tool. It combines small (nano), fast (short-pulses) and powerful (hard) necessary features for above complex investigations. FELs apply the principles responsible for synchrotron radiation to generate beams of laser-like light. There are existing several such research facilities located around the world [6]. Some of them are already built, taking an upgradation, processes and others are under the development or, even only in the planning phase. European infrastructure contributes at this network with several modern facilities [7].

SwissFEL, belonging to Paul Scherer Institute (PSI) is a very stable, compact and cost-effective X-ray FEL facility driven by a low-energy and ultra-low-emittance electron beam travelling through short-period undulators [8]. The facility consists of two X-ray beamlines ATHOS (soft) and ARAMIS (hard), respectively. ARAMIS [9] is successfully operating the first two hard x-ray experimental stations named Alvira and Bernina. A new branch (ARAMIS 3) or, alternatively Cristallina, is currently under the full realization. Mainly, it delivers ultra-short (sub-femto) hard X-rays (1.77-12.4keV) pulses to Cristallina (Cr) experimental station, for condensed matter physics research purposes.

By utilizing diffraction-before-destruction technique, new dedicated instruments located here will be focused on quantum phenomena (multibody) investigations. In this respect, a call for interest, including the development of two dedicated diffractometers (Dm), working with large delicate experimental instruments to create extreme sample environmental conditions (high magnetic field, low temperature) has been released [10].

The associated aspects of the challenging work, taken in to account the requirements, concept, design, manufacturability and precision for the final released products (prototypes) are presented below.

2. Diffractometers platform

Diffractometers (Dm) are specific X-ray instruments which allow to perform diffraction experiments, using various types of techniques and samples. A large variety of typo-dimensions has been developed since their introduction. Shortly, Dms could be for general or specific purposes. Subsequently, standard (universal) and customizable types are available.

Heavy load diffractometers are built to manipulate samples bigger than 100 kg. One of the companies is well known for producing high precision and reliable such products [11]. In addition, an experience for developing Dm(s) in an integrated platform already existed [12].

A set of two heavy load high precision Dm(s) have to alternatively work inside of the (Cr) experimental station, using the same beamline. The first, Dm (CrQ-Dm_1) is aiming to manipulate a heavy load sample environment (1t) and the second (CrQ-Dm2) smaller one (<0.5t). However, due to the complexity of the instrumentation to be prepared before experiments, the amount of time is large. A nearby preparation area is allocated inside the experimental station, and both Dm(s) will be permanently located here. This area has adequate means (crane) to manipulate Dm(s) instruments and their components.

Each of the diffractometers have to be easily moved/removed from/in the allocated area and down/upstream along of the beamline to reach the points of interest (focal points). The granite floor (90m^2) is adequate prepared (flat <500µm).

In the working position, Dm(s) are to be connected (docked) with a fixed rails along the beam line, through dedicated boards.

In order to increase the flexibility of Dm(s) use, the compatibility between both Dm(s) have to be assured, and with the third (Dm) located nearby, guaranteeing an easy and fast time of different set-ups or replacements.

3. Diffraction machines

Both, Dm(s) are mainly used in the horizontal diffraction geometry, which means that the investigation surface of the sample will be horizontal.

The first diffractometer (CrQ-Dm_1) is dedicated to manipulate the sample, working under special conditions: a) high magnetic field (5,2 T) and b) low temperature (<-10mK). A cryo-magnet (W_{M1}=650kg) with a considerable number of utility lines and flexible vacuum hose, being of large size (a_{M1}xb_{M1}=1150mm, h_{M1}=2.5 m) has the mass center (yC_{M1}=1.3m, xC_{M1}=zC_{M1}=30 mm) out of the rotation axis (Δ_R).

The second diffractometer (CrQ-Dm_2) will mainly manipulate a pulsed-magnet, having smaller weight (0.45t) and relative symmetric in-plane mass center (yC_{M2}=0.4m) producing pulsed magnetic field (50T) with a repetition rate (10-30 min). However, other setups are expected to be possible mounted for the general-purpose investigations.

Both, heavy loads Dm(s) which the architectures could be similar, relying on a similar planar transport system (air pads).

The exchange possibilities of the components between Dm(s) is provided and extended to a previously developed Dm (XPP-GPS) from Bernina endstation. However, due to the beam height limitation and non-magnetic requirements, Dm_1 is not using a sample goniometer stages for the tip/tilt motions.

Note: For some scattering experiments, a long flying vacuum tube (≈5m) with in vacuum detector is expected to join the Dm(s) at a later time, as well.

3.1. Kinematic Motions

Taking in to account the above specific requirements (individual and global), the proposed Dm(s) kinematic structures are presented below. As easy can be seen from Fig.1, (Dm_1, Dm_2) configurations are quite similar, but with significant differences.

Each of the Dm structure consists of a common supporting table (Tb), hosting different types of samples (Sp_1, Sp_2) and detectors (Dt_1, Dt_2) motion subsystems. Each of them can be seen, as a combination of a) in-series and/or b) in-parallel single (linear/rotation) motion axis. Dm(s) standing as a multi-degrees of freedom (MDOF) complex system.

A heavy load table (Tb), supporting (Dt) and (Sp) has to allow a roughly (pre-alignment) motion, regarding the beamline axis. Thus, a combined (series-parallel) kinematic device provides two(2) degrees of freedom (dof) of translational type (2T). The parallel one is responsible for the vertical motion (TY_T) through four(4) actuated jack devices. Stacked on it, a device is providing the horizontal motion (TY_T). In addition to these coarse travel motorized axis, short precision motion option exists, as well. This is based on small travel (TY'±15mm) screws, manually actuated. Note: By this, small (±0.5°) orientation motions (RX_T,RZ_T) are also possible. By this, (Tb) subsystem became of the 2T-(2R) type.

Note: Sseveal pairs of pads (air) permit a large planar motion (TX_P,TZ_P) on the floor.

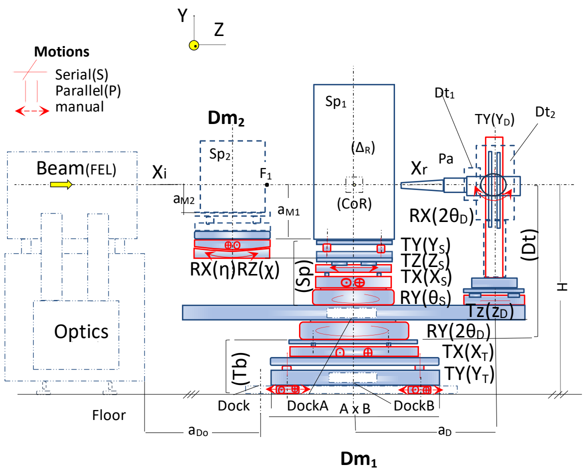

Figure 1. CrQ-Dm(s) kinematic motions and integration

Generally, a samples (Sp) subsystem must precisley pose (position & orientation) the samples (magnets & instruments) towards the incoming beam (X_i). (Dm_1, Dm_2) include a combination of serial devices, performing high precision motions of positioning. In addition, in an earlier stage, it has to position rotation center (CoR) of Dm(s) – C (Dm_2) or axis (Δ_C) (Dm_1) of the machines to coincide / intersect with the focal point (F) /axis of the beam line (alignment). Note: The nominal value of the beam height is set up at fixed height (H=1380 mm).

In the first case (Sp_1), a basic fully rotational motion (RY) device, horizontally mounted is combined with other three ones, providing translational spatial (TX,TY,TZ) short motions of positioning. The fixing area being large enough (A_{XZ}= 400x400 mm. By this, (Sp_1) as a whole will have four (4) dof (1R-3T).

In the second case (Sp_2), short stroke angular rotations (RX) and (RZ) around the planar axes (X,Z) have to be performed by a compatible device interposed between (TX,TY) and (TZ) from above. The virtual rotation points of each have to coincide with C(CoR), whole subsystem becoming of 5dof (2R-3T) type.

Note: An option to use a single device, based on Parallel Kinematic Mechanisms (PKM) [14] for positioning the samples, e.g outsourcing (hexapods) or, in-house (quadropods) has been also investigated, due to their already proved advantages (load, precision). However, the stacked use routine prevailed against any of these compact but complex motion devices (Note: HP/QP are 6dof devices of 3T-3R types).

Detector (Dt) subsystem have to provide enough dof(s) motions to pose two different) pixel detectors (JUNGFRAU, PSI): a) Dt_1 (8M, 40kg, 300x300x400 mm) and b) Dt_2 (1,5M, 10kg, 200x400x120 mm), in the right position relative to the refracted rays (Xr). Therfore, Dt(s) consists of an orthogonal in-series combination of: a) basic two(2) - rotation device (RY, $2\theta_H$) and translational (T_{ZD}, Z_D=400mm) common devices and b) optional - rotation (RX_D, $2\theta_V$=±20°) and translation (TY_D, Y_D=±400mm), in the case of (Dt_1). By this, (Dt_1) is of 2R-2T and (Dt_2) as R+T types.

Note: A polarization analyser (Pa, m=25kg) is expected to be latter combined with (Dt_1), as well.

An overview of most important types of motions, including the range and precision parameters are provided in the Table 1. The afferent circles Ci, i=1-4(5*) for the CrQ-Dm_1 (1S–2D) and CrQ-Dm_2 (3S–2*D) *-optional structures are included, as well. The speed range (min-max) for a simple T/R motion have to be between 0,005-0,5 mm/s and 0,005-1 °/s.

Note: A general (beam) right-hand coordinate system of reference (OXYZ), having Z-axis along the beam (+ from optics) and the vertical perpendicular Y-axis (+, ascendent) and local (machine) system oxyz with the origin (o) in the center of rotation (CoR) have been adopted. However, in the text, for the simplicity, sometimes the interchanged letters applied.

Table 1 CrQ-Dm(s) motion parameters

Type (T) (R)	Range [mm] [°]	Acc. [μm] [arcs]	Rep. [μm] [arcs]	Circles (Ci) i=1-n
RY(θ_{Sp})	±180	1	0.36	C1$_S$(μ)
RX(θ_{Sp})* RZ(θ_{Sp})*	±10 ±10	1 1	0.36 0.36	C2$_S$(η) C3$_S$(χ)
RY($2\theta_{DtH}$) RZ($2\theta_{DtV}$)**	±180 ±25	1 3	0.36 1	C1$_D$(ν) C2$_D$(δ)
TXZ(X_{Sp},Z_{Sp}) TY(Y_{Sp})	±25 ±10	1 1	≤1 ≤1	- -
TX(X_t) TY(Y_t)	±60 +60-30	4 4	2 2	- -

* - Dm2, only, **- optional (Dm_2)

3.2. Design Concept

The whole products has been divided in three– a) table (Pm_1), b) sample (Pm_2) and c) detector (Pm_3) main modules, Fig.1.

Each of the Pm(s) included several simple standard/ customized specific heavy loads and high precision positioning units (Pu_i), i=1-7 with high level of compatibility between them, offering the advantages of high reconfigurability.

Note: The increased structural compatibility is acting on both, mechanical and electrical parts (motors, encoders, control), as well.

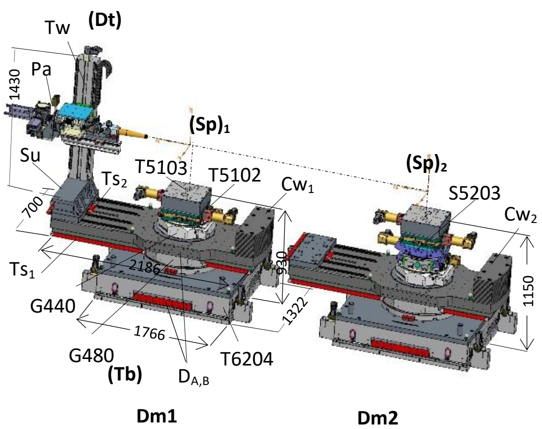

Figure 2. CrQ-Dm Layout 3D view design (CAD)

The first positioning module (Pm_1) corresponds to the supporting table (Tb) subsystem. It was designed based on a standard type component (Tb6204), providing stiff and stable support and precision (pre)alignment motions for all the necessary working modules (Dt and Sp) above. It consists of two integrated motorized components: a) table itself unit (TY_T) and b) integrated stage (rails and motor) (TX_T) Pu(s). It has four(4) powerful driving jacks and gear boxes fixed on a strong base, vertically moving a second plate(table). In addition, (Pm_1) has been provided with three (3) pairs of large air pads for the planar transport, before it will be docked through Dock A at the fixed docking station. Note: Dock B is fixed on (Dt) arm. Due to the allocated space constraints reasons, the pads are not exceeding the plane size of the (Tb), being also covered by shields.

Sample modules (Sp_1, Sp_2) consist of several stacked Pu(s) of linear and/or rotation types components, forming (Pm_2) modules. The basic one is a heavy load and precision gonio stage (G440), holding an integrated planar one (T5102). On top of them, a vertical translation stage (T5103) is fixed in the (Sp_1) case. For (Sp_2) an additional powerful segment stage (S5203) is used to perform tip/tilt precision arc (short) motions. (Sp_1, Sp_2) positioning devices have similar characteristics (power, size, stiffness) and the centering/fixing pattern holes, which are identical with XPP-GPS (Bernina), excepting the load capacity.

Note: A design effort was taken to define and minimize the (M_1) maximum torque for G440.

Detector modules (Dt_1, Dt_2), forming (Pm_3) module were built to accomplish with the required support and motion specific conditions for the detector products. It is based on a powerful motorized goniometer (G408) and a stiff symmetric arm, holding a very stable (4x guides) horizontal stage (T5101), moving a vertical heavy tower (Tw), in the (Dt_1) case. Basically, (Tw) includes a stiff base (support), holding a long vertical (TY_D) stage which moves a rotation (RX_D) stage which hold a JUNGFRAU (Dt) or Polar analyser (Pa) submodule.

Note: Due to the tight space restriction, efforts have been done to design a symmetric shape (Dt) arm, increasing its rotation angle and not affecting its stiffness.

From the control point of view, a positioning drive system must be able to move the final mechanical element (e.g. stage) at desired position with required accuracy and speed.

Generally, most of the motorized axis are using servo motors (AM8121, BECKHOFF), gear boxes (Gb2000), limit switches (24V/NC) and absolute encoders - head (RESOLUTE) and tapes/ring (RKLA / RESA) types from RENISHAW controlled in a closed loop way. All encoders are compatibles with BiSS-C or SSI communication protocol (26-bit).

The control of motion is performed via an Ethercat-based solution (BECKHOFF) and EPICS software tool.

As Dm(s) are often moved, cable minimization was a "must" design issue. As such, a motor control box was integrated on each Dm(s) (not shown in Fig.2).

Note: To avoid unexpected collisions (optics) and between components, touch sensors Ts1, Ts2 (TS28/TAPESWITCH) have been included (Dt), from safety reasons.

An overview of the selected Pu(s) components, for each of the motion axis (Ai, i=1,…,13) belonging to the basic modules is provided in Tab.2.

Table 2 CrQ-Dm(s) motion axis components

Axis (Ai)	Module (Pm)	Unit (Pu)	Gear (i)
A1-A4 A5	Tb	T6204	5 10
A6 A7	Dt	G480 T5101.80	20 5
A8 A9,A10 A11*, A12* A13	Sp	G440 T5102.50 S5203.50 T5103.C40	20

* - Dm_2, only

3.3. Precision

In the first step, a basic set of Dm(s) have been manufactured, another (optional) components, being intentionally delayed, and scheduled for a later time.

Most of the customized components were based on the company`s standard or customized products, where in-house a non-magnetic knowledge and experience already existed.

However, care has been taken for all steps, starting with the selection of materials (stainless steel, Al, brass, etc) and their manufacturing process, to assure the final prescribed precision.

In the machining process the procedures involved the machining of sensitive interconnected surfaces (basic plates, interfaces, etc) belonging to key elements (stages, guides, etc) with high quality (Ra=1,6) and suitable dimensional tolerances, assuring the adequate geometric errors of motion axis(││,┴).

In the assembly process, care has been taken to adequate mount the components and align them in the subsystems (modules), with a reproducibility of max. 20 µm, for both horizontal and vertical arrangements. The centering means (holes/pins) have been often used. In addition, adequate clamps mounts for electrical/air cables and water pipe provided, as well.

In the transportation/packaging operations, each of the heavy components did not exceed the max. crane load capacity (1.6t), being suitable balanced with fixture and hooks (Hk) for lifting.

In order to accomplish with the final required precision, all individual and combined involved positioning devices have been tested. The results have been included in a Factory Acceptance Test (FAT) report which will be soon released.

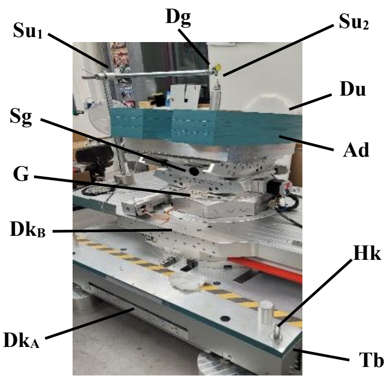

Figure 3. CrQ-Dm_2 prototype (tests)

The testing procedures consisted in to carefully determination of general or, functional (range, homing, collisions, etc) behaviour and precision parameters (accuracy, repeatability, resolution).

In an earlier step, all actuated individual components mentioned before, but especially rotation stages (gonio) have been tested from accuracy point of view and the results graphic represented (diagrams). The metrological setup included standard components as, interferometer (XM-60, RENISHAW), dial gages, levels, etc and customized artifacts (granite base, supports) and data manipulation (PC) means. In addition, stepping motors and a dedicated in-house control box (SMC9000) have been used. Note: Even each linear/rotational $(Pu)_i$ are equipped with (absolute) encoders to determine the position of the mobile elements with high resolution, a calibration process was sometimes necessary to compensate for the mechanical systematic errors.

In the final step, the global precision parameter - Sphere of Confusion (SoC) has been evaluated. Even if (SoC) represents all the accumulated errors of the machine moving around the center of rotation (CoR), during the combined motions (Sp, Dt), in our case is working for Sp $(SoC)_S$, only. For a customer preferred configuration, an example is given In Fig.3. It consists of a (Dm_2) combination of two(2) positioning stages - Gonio (G) and Segment (Sg), supporting through an adapter plate (Ap), the dummy (Du) load. The measurements have been performed with a dial gage (Dg) hold by a support (Su_1) and a calibrated ball Grade 5 (Ø=14mm, e<±0.5µm, ○=25nm) fixed in an adjusting head (H1002) hold on a vertical support (Su_2). (SoC) was evaluated in two cases, a) without and b) with load (Du_1=1000kg /Du_2=750kg). A comparative view of the requested and obtained values is given in Tab. 3. $(SoC)_{S1}$ represent a runout error of rotation axis of each individual stage. $(SoC)_{S2,3}$ represent a combination of two(2) or three(3) runout errors of the stages.

Table 3 Dm2 runout - errors (SoC)

<table>
<tr><th>SoC_i [i=1,2]</th><th>$RY(2\theta_D)$ [µm]</th><th>$RY(\theta_S)$ [µm]</th><th>$RX(\eta_S)$ [µm]</th><th>$RZ(\chi_S)$ [µm]</th><th>Note</th></tr>
<tr><td>$(SoC)_1$</td><td>4 (6)</td><td>1 (5)</td><td>6 (6)</td><td>6 (6)</td><td rowspan="2">$(SoC)_{S1}$</td></tr>
<tr><td>$(SoC)_1^*$</td><td>6 (12)</td><td>2 (10)</td><td>6 (15)</td><td>15(15)</td></tr>
<tr><td>$(SoC)_2$</td><td colspan="2"></td><td colspan="2">14 (20)</td><td rowspan="2">$(SoC)_{S2}$</td></tr>
<tr><td>$(SoC)_2^*$</td><td colspan="2"></td><td colspan="2">20 (35)</td></tr>
<tr><td>$(SoC)_3$</td><td></td><td colspan="3">21 (25)</td><td rowspan="2">$(SoC)_{S3}$</td></tr>
<tr><td>$(SoC)_3^*$</td><td></td><td colspan="3">24 (40)</td></tr>
</table>

* - Load

As resulted from above, the partial $(SoC)_{S1}$ and combined (SoC) values are at most equal with the maximum accepted ( ) values.

Note: In the Site Acceptance Test (SAT), the exact pose (position and orientation) of (Dms) along the beamline, a laser tracker is recommended to be used. Especially, the horizontality of the supporting table and the detector arm rotational motion must be checked. In this respect, some fiducials markers have been allocated. Each of them consists of a central piece (reflector ball, Ø=35.7mm) and the adequate interface (M8).

4. Conclusions

A set of two dedicated heavy load precision diffractometers (Dm_1, Dm_2) for the actual stringent specific investigations of advanced quantum materials (QMs) have been developed. (Dm_1) and (Dm_2) have been fully integrated in a single working platform (CrQ-Dm), exhibiting high flexibility and compatibility features (inside/outside). The challenged work with both, extreme load and precision, proved to be successfully one. After the necessary performed tests, both Dm(s) machines in the basic configuration have been delivered, waiting for the next installation and commissioning steps. With this fast development pioneering work, breakthroughs investigative results are expected to be shortly done. In the next paper, more detailed results related with the obtained precision will be presented.

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