ISBN: 978-3-95450-207-3 doi:10.18429/JACoW-MEDSI2018-WEOPMA03

APPLICATION OF ADDITIVE MANUFACTURING IN THE DEVELOPMENT OF A SAMPLE HOLDER FOR A FIXED TARGET VECTOR SCANNING DIFFRACTOMTER AT SwissFEL

Xinyu Wang†, Jan Hora, Patrick Hirschi[1], Haimo Jöhri, Claude Pradervand, Bill Pedrini,
Paul Scherrer Institut, 5232 Villigen, Switzerland
[1]also at HELVETING Engineering AG, Neuenhof, Switzerland

Abstract

Whilst the benefit of additive manufacturing (AM) in rapid prototyping becomes more and more established, the direct application to 3D printing is still demanding. Exploitation of AM opens the door for complex and optimized parts which are otherwise impossible to fabricate. Therefore, consistent efforts are currently directed to gain specific knowledge on the numerical simulation and the design process.

For a vector scanning diffractometer foreseen for fixed target protein crystallography at the Swiss X-ray free electron laser (SwissFEL) [1], we developed, manufactured and tested a 3D-printed sample holder with carbon fibre reinforced polyamide material. The diffractometer serves to collect diffraction patterns at up to 100 Hz rate on many small protein crystals (< 5 µm) by scanning the sample in the X-ray beam following the custom trajectories. The large accelerations in the motion plane transverse to the beam require the holder, which is tightly fixed on the diffractometer stages, to be particularly light and stiff.

Our work on the design and the dynamic tests for the 3D-printed holder is presented here. For sake of comparison, the numerical analysis and tests were extended on a CNC-machined aluminium holder realized to fulfil the same function.

INTRODUCTION

The collection of X-ray diffraction images with the fixed target protein crystallography instrument SwissMX [2], currently under realization at SwissFEL, relies on scanning the sample in the X-ray beam using an advanced diffractometer with translation axes in *x*- and *y*-directions (Fig. 1). In the specified error budget of 1.2 µm in total between the impact position of a femtosecond SwissFEL X-ray pulse and protein crystal position, the contribution from the deformation of sample holder is restricted to be less than 200 nm. The benchmark motion of the stages is sinusoidal with 50 Hz frequency and a maximum acceleration of 2.5 m/s^2, corresponding to a motion amplitude of 25 µm. The weight of the sample holder is crucial due to the large accelerations acting on the moving parts. The total mass allowed by the performances of the stages must be below 100g. Given the weight of the sample unit of 30 g (including sample chip, sample pin and pin-holder magnet), the sample holder maximal weight is 70g. The natural frequencies of the sample holder have been requested to be above 400 Hz.

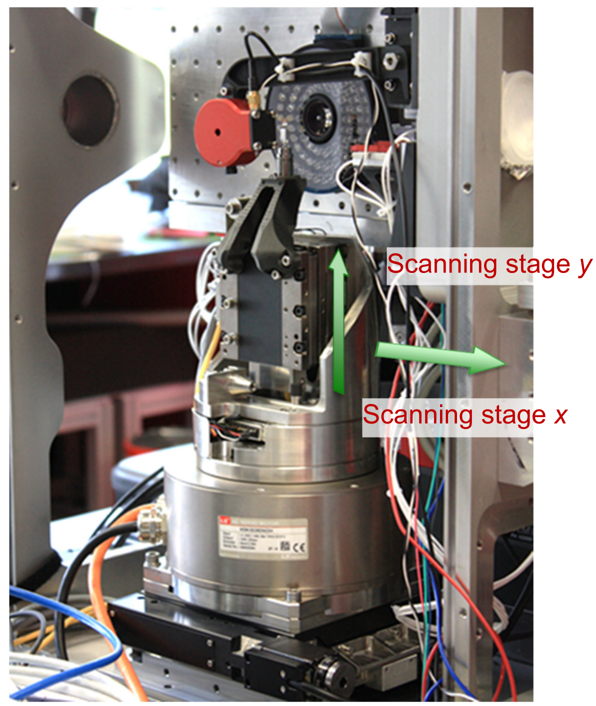

Figure 1: Sample diffractometer with sample holder and sample chip.

DESIGN OF THE SAMPLE HOLDER

To realize the sample holder, we considered both possibilities of aluminum material, i.e. by traditional CNC manufacturing, and by 3D printing with carbon fiber reinforced polyamide. In the Continuous Filament Fabrication (CFF) printing process, endless carbon fibers are printed layer by layer in predefined orientations and embedded in melted polyamide matrix material ([3]) to achieve high stiffness and low weight. The lack of material data for general 3D printing application limits the numerical predictions of the dynamical properties. In Table 1, material properties are given for uni-directional (UD) fibre orientation and for matrix material. UD composite shows the highest

† xinyu.wang@psi.ch

ISBN: 978-3-95450-207-3 doi:10.18429/JACoW-MEDSI2018-WEOPMA03

stiffness but only in the direction of the fibres and is anisotropic. The more common composites with fiber orientation in 0°/45°/90°-directions have lower stiffness, but has the advantages of being quasi isotropic and showing higher shear strength.

Table 1: Materials Properties [3]

	Alu	Carbon Pomposite UD	Micro-Carbon Reinforced Polyamide
Density [g/cm^3]	2.7	1.4	1.2
Tensile modulus [GPa]	70	54	1.4
Bending modulus [GPa]	70	51	2.9

Topology Optimisation

Since the introduction of topology optimisation (TO) theory in 1988, many algorithms have been rapidly developed [4]. With additive manufacturing, more and more complex shapes can be realized. TO is the key feature for form-finding of optimized geometry. Recently, TO has been integrated into many existing CAD and CAE environments. Thus, in addition to providing ease in the transition of results and geometries between TO and finite element (FE) analysis, the further advantage is that all features and functionalities of reliable finite element (FE) solver are made accessible to TO. The TO and FE analysis reported here has been performed with ANSYS workbench Release 19.

The design space was defined after a collision analysis in CAD (Fig. 2a). In the final design of the holder, the goal was to occupy 25% of the volume with a part of highest stiffness and highest natural frequencies. Constraints were defined at bolted connections to stage, kept fixed in the model. The pin and the sample chip were defined as a point mass located at the gravity center. The first analysis aimed to maximize the first natural frequency, which resulted in the geometry shown in Fig. 2b. Because of the motion is both in x- and y-directions, also the second mode is relevant, and therefore further optimisation was carried out to maximize both the first two natural frequencies. The new obtained geometry is illustrated in Fig. 2c. Further consideration was devoted to the static stiffness under acceleration of 2.5 m/s^2 in both directions. Figure 2d shows the output design with two static loads of equal weight factors.

For general applications with multiple requirements, TO leads not only to sole optimum, but to many optima. Giving consideration of all requirements to possible weighting factors leads to a threshold of optimized regions, and leaves a freedom of design to engineers. The optimization results are only as good as the definition of objectives (goals, responses) based on specification. Before a TO solution is accepted, the design has to be validated by FE analysis.

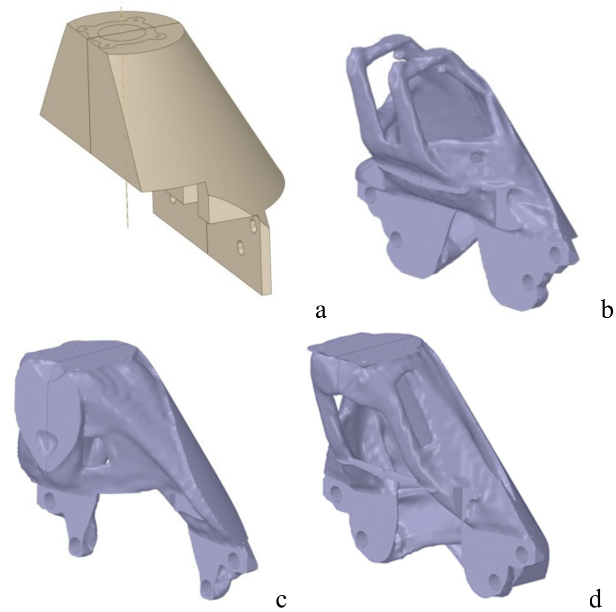

Figure 2: Design space for the stiffness optimization (a) and optimized structure (b, c, d).

Simulation to Design

The simulation employs body-fitted Cartesian all-hex meshing which is especially suitable for 3D printing simulations. Figure 3a shows the retained elements after TO of the most regular final geometry. Figure 3b shows the smoothed geometry from STL cleanup, which still requires a lot of fine tuning to make it eventually suitable for direct printing.

The final design is based on the compromise that the sample holder is both CNC manufacturable and 3D printable (Fig. 4).

ISBN: 978-3-95450-207-3 doi:10.18429/JACoW-MEDSI2018-WEOPMA03

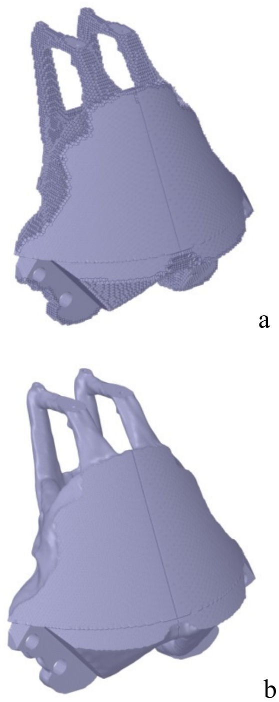

Figure 3: Retained elements (a) and smoothed geometry (b).

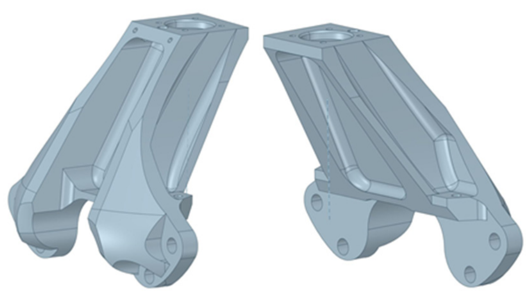

Figure 4: Final design geometry.

Design Validation

FE analysis has been performed for design validation with both aluminium and UD carbon fibre composite materials. A summary of the results for static and natural frequency analysis can be found in Table 2. The aluminium part has a weight of 64 g and is just within the specification. The carbon composite part of 33 g weight is much lighter. Figure 5 shows the deformation patterns of the aluminium part under vertical and horizontal accelerations of 2.5 m/s^2. Deformations for both load cases and with both materials are below 32 nm, thus well within the specified 200 nm. Figure 6 shows the shape of the first two modes: the first is a vertical bending mode, while the second is a torsional one. The first natural frequency of aluminium sample holder is 790 Hz, and of UD carbon composite is 713 Hz. With both materials, the requirement of the lowest natural frequency to be above 400 Hz is achieved. Due to the lack of material data of carbon fibres in general orientation, the calculation was performed based on stiffness of UD composite in fibre direction which is higher than that achieved in the real production. The final deformation of the 3D printed sample holder is therefore expected to be higher and the natural frequency to be lower than calculated due to material property deviations.

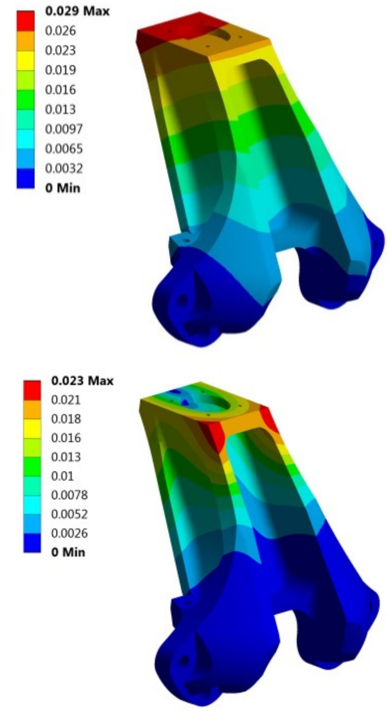

Figure 5: Deformation [µm] of the aluminium part under vertical (upper) and horizontal (lower) acceleration of 2.5 m/s^2.

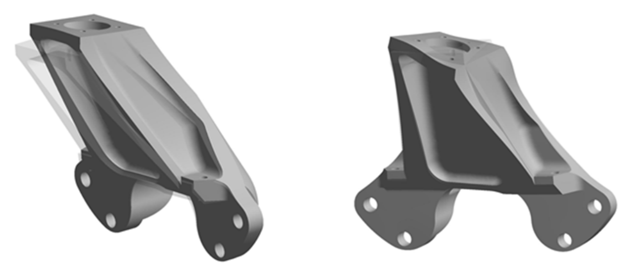

Figure 6: Mode shapes of the 1st and 2nd modes.

Table 2: Summary of FEA Results

	Aluminium	**Carbon Composite UD**
Weight [g]	64	33
Deformation [nm]		
Vertical	29	32
Horizontal	23	30
Natural frequency [Hz]		
f_1	790	713
f_2	1350	1206

ISBN: 978-3-95450-207-3 doi:10.18429/JACoW-MEDSI2018-WEOPMA03

DYNAMIC TESTING

A modal shaker (Mini SmartShaker TMS K2007/E01) was utilized to apply the appropriate acceleration of 2.5 m/s^2 at 50 Hz for a qualification test.

The sample holder was mounted via an adaptor to the shaker. For the vertical excitation, two tri-axial accelerometers (PCB 356B18) were used: one was placed on the adaptor and the other on the sample holder (Fig. 7). The accelerometer with the joining plate had a weight of 30 g, corresponding to the total mass of pin-holding magnet and pin. The input acceleration is recorded by the accelerometer on the adaptor, and the output acceleration is measured by the accelerometer on the sample holder. For the transversal motion, the adaptor was rotated to the vertical direction (Fig. 8). Two 3D printed sample holder parts were tested simultaneously to prevent the out-of-axis motion due to eccentric mass centre. The input signal to the sample holders was recorded by an impedance sensor PCB 288D01 on the top of adaptor.

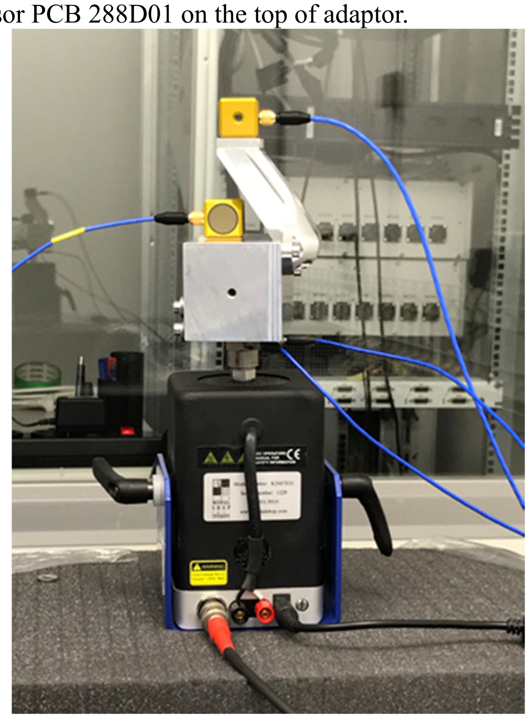

Figure 7: Vertical dynamical test setup with aluminium sample holder.

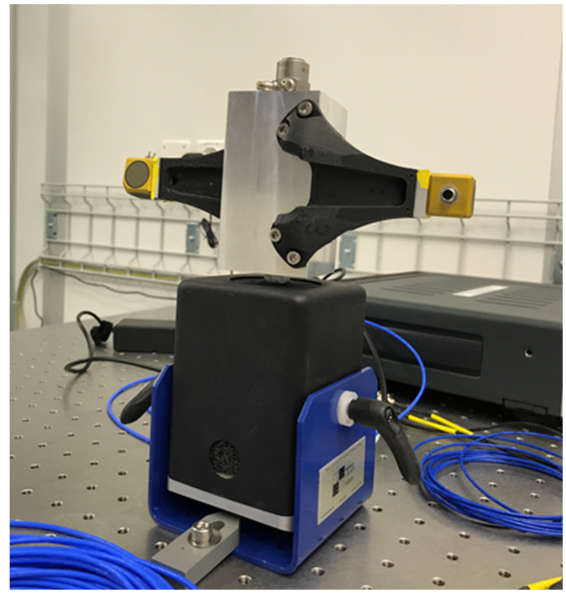

Figure 8: Transversal dynamic test setup with two composite sample holders.

The response of the following four sample holders under forced harmonic vibration was investigated:

- M1: 3D printed micro-fiber reinforced polyamide
- M2: 3D printed carbon fiber composite with quasi-isotropic orientation, printed from the curved back side
- M3: 3D printed carbon fiber composite with quasi-isotropic orientation, printed from the flat front side
- M4: Aluminum

The shaker was set to a harmonic motion at 50 Hz with a maximum acceleration up to 3.3 m/s^2. The phase shift of the output and input was calculated from cross spectrum functions. Figure 9 depicts a 3D color map of the phase as a function of time on the vertical axis and frequency on the horizontal axis, with phase value encoded in the color corresponding to the scale on the left of the picture. As the forced vibration excitation is at 50 Hz, the phase shift is correlated at this frequency. Beyond the excitation frequency, the phase information has no physical meaning, and therefore no correlation can be found.

ISBN: 978-3-95450-207-3 doi:10.18429/JACoW-MEDSI2018-WEOPMA03

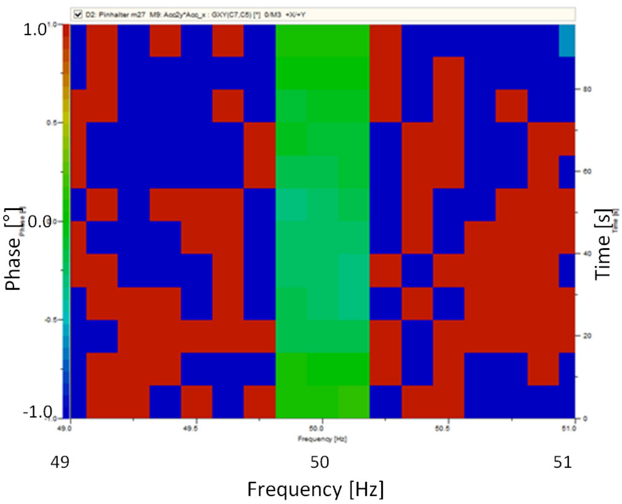

Figure 9: Color map of phase shift from 49 to 51 Hz.

Table 3: Summary of Measurement Results

	Aluminium M1	Composite M2/M3
Weight [g]	63	40
	Vertical excitation	
Phase [°]	0.16	0.36
Pos. Error [nm]	70	157
	Transversal excitation	
Phase [°]	-	0.31
Pos. Error [nm]		135

The phase shifts tested at various amplitudes with accelerations up to 3.3 m/s^2 are scaled linearly to the acceleration of 2.5 m/s^2. The main measurement error is the off-axis motions resulting from the tilting of the shaker output mounting, which is restricted to be below 10% of the axial motion amplitude. With the sample stage the tilting motion can be eliminated, and the measurement with the shaker corresponds to a worst case behaviour of the sample holder. A summary of the measured phase shifts is given in Table 3.

The aluminium sample holder has the lowest phase shift of about 0.16°. The two composite parts printed from different sides and therefore with different support structures behave similarly, with phase shift around 0.36°. The maximum position error related to 0.36° phase shift at 25 µm amplitude is estimated to be

$$25\ \mu m * \sin(0.36°) = 0.157\ \mu m.$$

The error is therefore within the 200 nm specification. For the aluminium holder, the position error estimate (0.16° phase shift giving 70 nm) is even lower, but the part is 50% heavier. The micro-fibre reinforced polyamide part has a phase shift of more than a factor of four larger, resulting in a position error of 600 nm which is too high for practical use.

CONCLUSION

Topology optimisation plays a key feature in advanced manufacturing. Its application is not only beneficial to 3D printing but also to traditional CNC manufacturing.

In the case of the sample holder considered here, the design resulted from the compromise of both CNC machinable and 3D printable. Holders made with aluminium and endless carbon fibre reinforced composites turned out to qualify for the foreseen application. Micro-fibre reinforced polyamide was too soft, with the holder exhibiting a phase shift four times larger than the part with endless carbon fibre. The aluminium part was the stiffest but 50% heavier. The 3D printed composite part was chosen as the preferred option for the fixed target protein crystallography diffractometer in the SwissMX instrument.

The lack of general material properties of carbon fibre composites material limits the numerical prediction possibilities of the mechanical behaviour of the parts. Further knowledge on material properties, influence of printing process still need to be gained.

ACKNOWLEDGEMENTS

We want to thank Peter Hottinger for the support in mechanical testing.

REFERENCES

[1] Christopher J. Milne *et al.*: "SwissFEL: The Swiss X-ray Free Electron Laser", *Appl. Phys. Lett.*, vol. 7, 720 (2017)

[2] SwissMX (former ESB-MX) concept design report, available at `https://www.psi.ch/swissfel/swissfel`

[3] MarkForged, Inc. & Mark3D GmbH: "Fertigung neu definiert", 04 2018.

[4] Ole Sigmund and Kurt Maute, "Topology optimization approaches, a comprarative review", *Structural and Multidisciplinary Optimization*, 48:1031–1055, DOI 10.1007/s00158-013-0978-6