COUPLING OPTICAL DIAGNOSIS INTO THE MFX XLJ CHAMBER

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INTRODUCTION

This project focuses on developing an optical diagnostic system for the Macromolecular Femtosecond Crystallography (MFX) instrument at LCLS. Many experiments at MFX rely on delicate samples, such as biological molecules in solution or microcrystals, which can degrade due to environmental factors before reaching the X-ray beam. Currently, users assess sample quality using external UV/Vis spectroscopy. This approach, however, does not provide real-time feedback during experiments.

The goal of this project is to design and implement a compact optical system that allows users to monitor samples immediately before interaction with the X-ray beam inside the eXchangeable Liquid Jet (XLJ) chamber.

CHALLENGES

- **Space Constraints**: The XLJ chamber is very compact, and any added components should avoid obstructing the X-ray beam path while coupling to the horizontal jet, which requires vertically oriented optics
- **Chromatic Aberrations**: The broadband light source causes the beam to focus at different points across wavelengths. The design must compensate for this to ensure accurate spectral measurements
- **Beam Size**: A very small focused beam is needed to match the size of the liquid jet and small biological samples

DESIGN OVERVIEW

- **Reflective collimators**: direct fiber-coupled light at a 90° into free space. A focal length of 7mm is used to ensure a compact design
- **Achromatic doublets** (f=19mm): achieve consistent focus across visible light range (400 to 700nm)
- **Multimode fibers:** 50µm core for input limits beam size and 600µm core for output maximizes light throughput to the spectrometer
- **Translation stage and post clamp:** offer three degrees of freedom for precise alignment with the jet

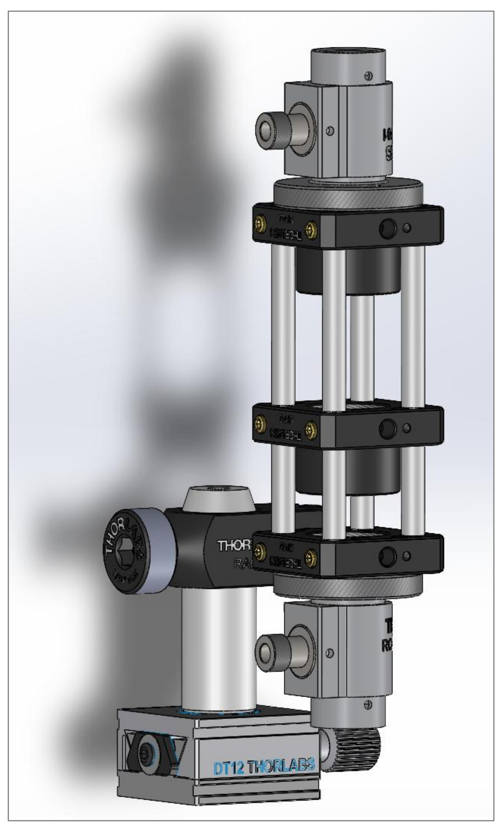

Fig. 1: CAD model of the optical system

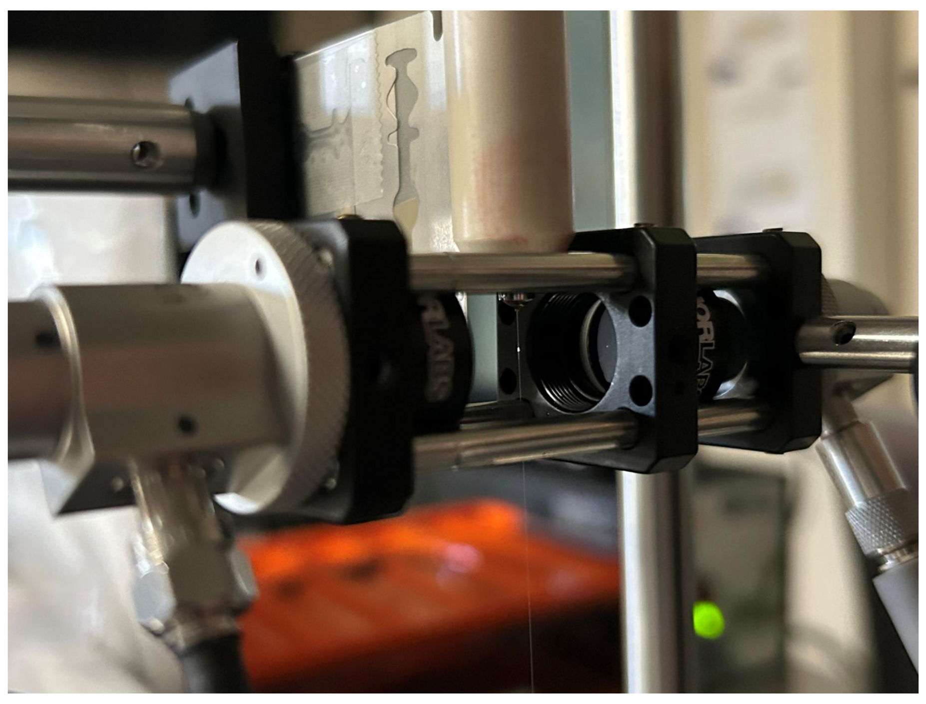

Fig. 2: The assembled optical system and liquid jet

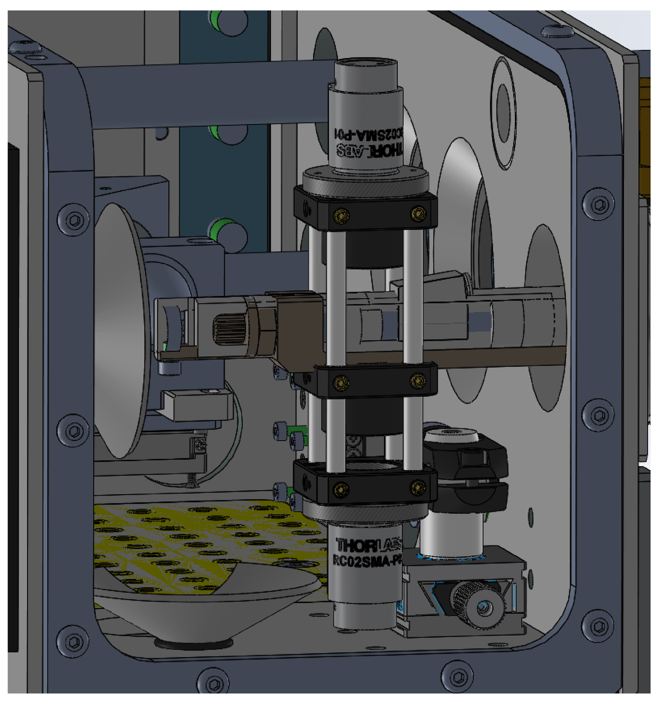

Fig. 3: CAD model of the optical system in XLJ chamber

BEAM PROFILING BY KNIFE EDGE SCAN

A knife edge scan was used to characterize the focused beam profile by translating a razor blade across the beam and recording the resulting intensity. The focused beam size was experimentally measured to be 83µm.

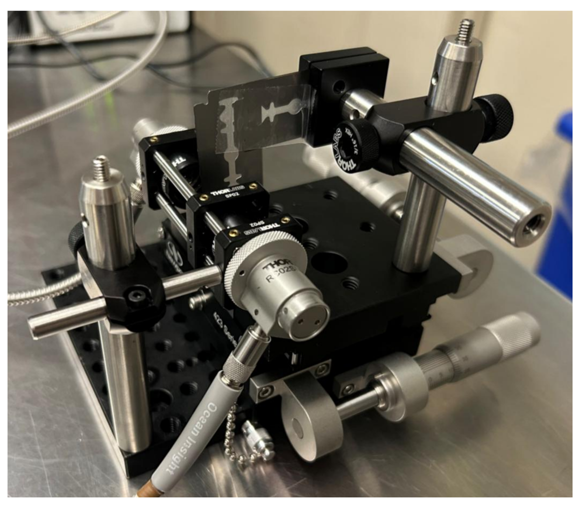

Fig 4: Experimental setup for knife edge scan

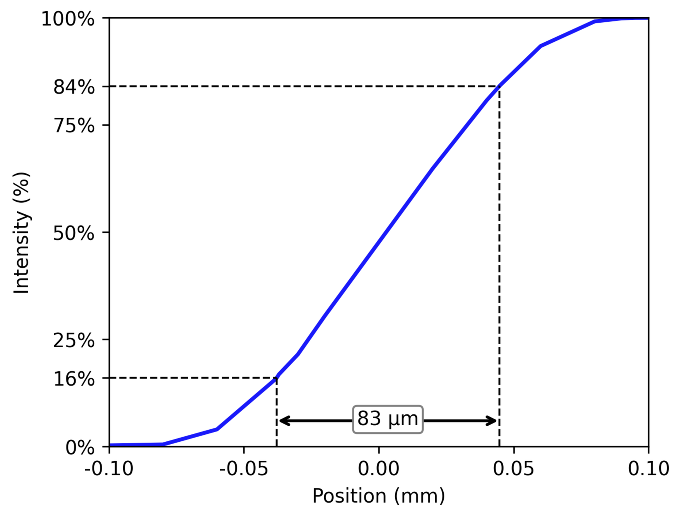

Fig. 5: Measured intensity versus knife edge position relative to optical axis

SPECTRAL MEASUREMENTS

To evaluate the performance of the optical system, spectral measurements were conducted on two sample solutions: water and $Fe(bpy)_3$, which were passed through a 100 µm liquid jet.

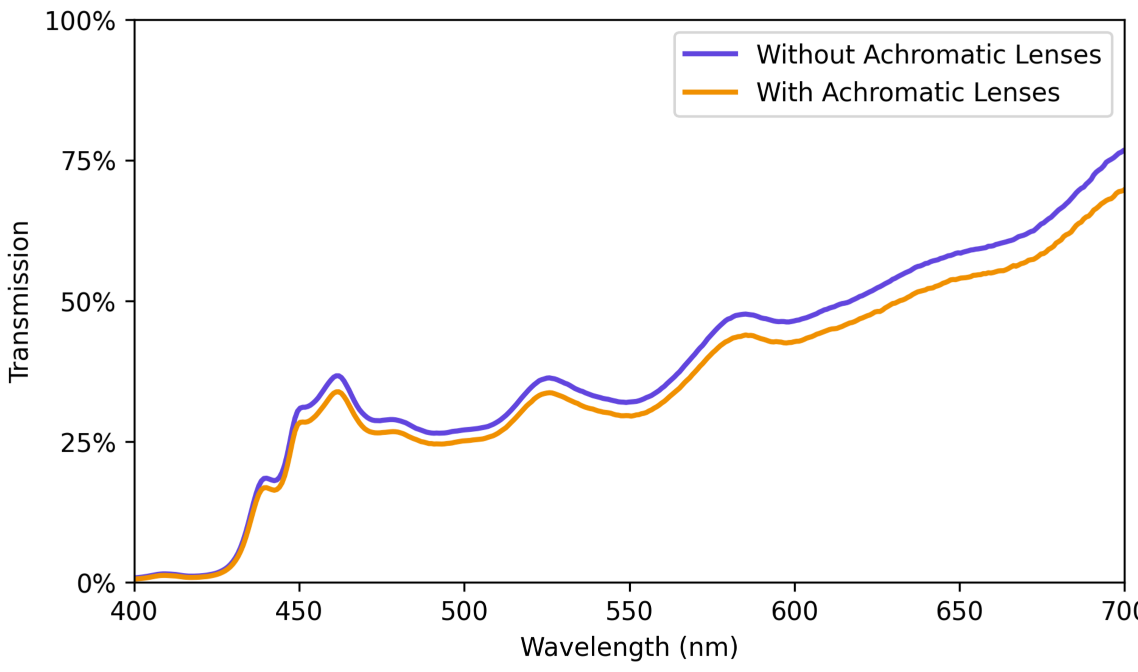

Fig. 6: Transmission through optical system
The beam is not perturbed chromatically by the addition of lenses.

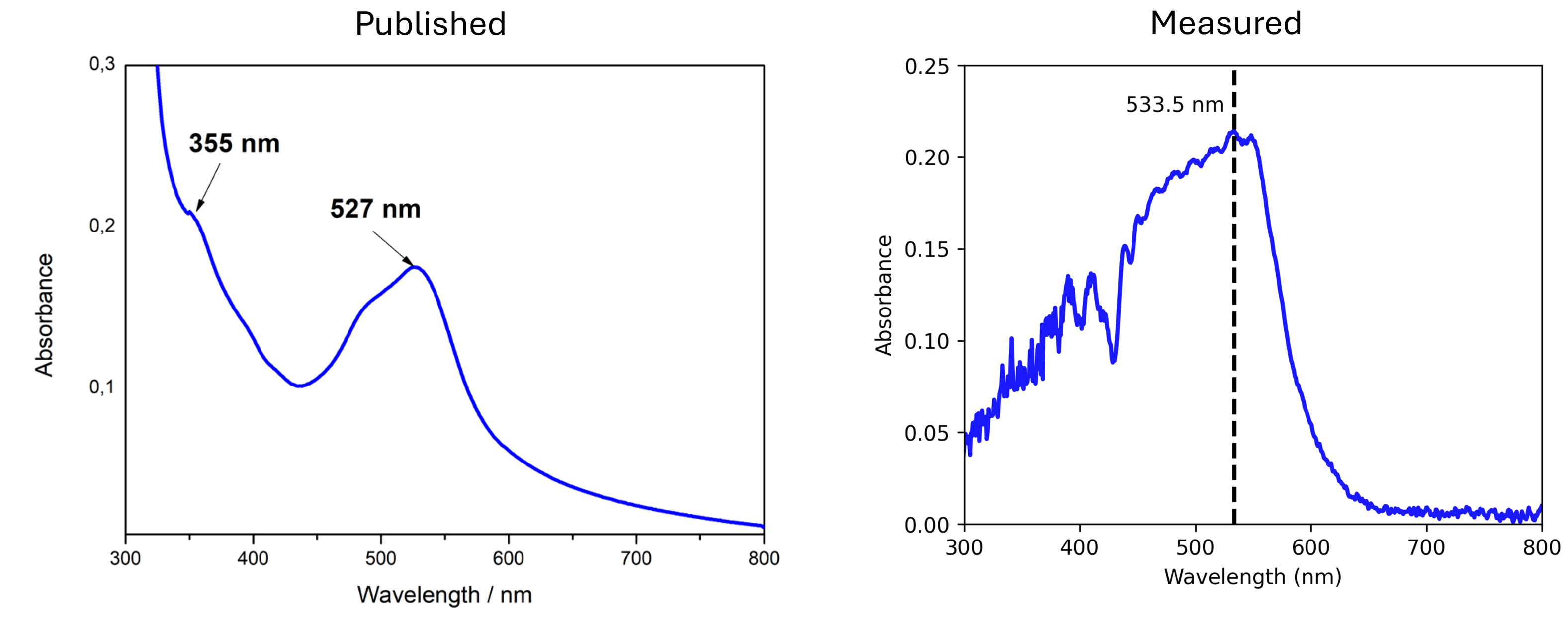

Fig. 7: Absorption spectra of $[Fe(bpy)_3]^{2+}$
The measured spectrum matches the shape of published data [1].

Future Work

1. **Reducing Spot Size**: Aim to reduce the optical beam spot size from ~80 µm down to 30 µm or even 5 µm, which is critical for biological microcrystals and smaller chemical samples
2. **Extending to the UV Range**: Current optics cover the visible spectrum. Future work includes developing a design for UV to broaden diagnostics for a wider variety of samples

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