NATIONAL ACCELERATOR LABORATORY

Optimizing and Characterizing Liquid Sample Jet Performance

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INTRODUCTION

FEL Pulses

LCLS is a **Free Electron Laser (FEL)**, generating hard X-ray pulses used to take atomic-resolution snapshots of samples. An FEL pulse is **ultrashort** (nanoscale wavelength), **ultrafast** (femtosecond timespan), and **ultra-bright** (a billion times the photon count in conventional synchrotron light). Altogether, the pulse is short enough to probe at the atomic scale and fast enough to pass through an intact sample before the beam intensity destroys it.

Since the FEL generates up to 120 pulses per second, destroyed sample must be replaced rapidly. We efficiently replenish sample using liquid sample jets. Here we collect preliminary data characterizing and optimizing the operation of cylindrical and sheet jets.

Jet Setup

At the beamline, sample is drawn from a reservoir, jetted in front of the FEL beam path, and funneled back into the reservoir. A fluorescence detector sits next to the setup, while a scattering detector sits above it. Together, the detectors catch the signal from each pulse "snapshot", allowing us to form the image of the sample that was hit.

We reconstructed the basic jet setup outside the beamline for testing:

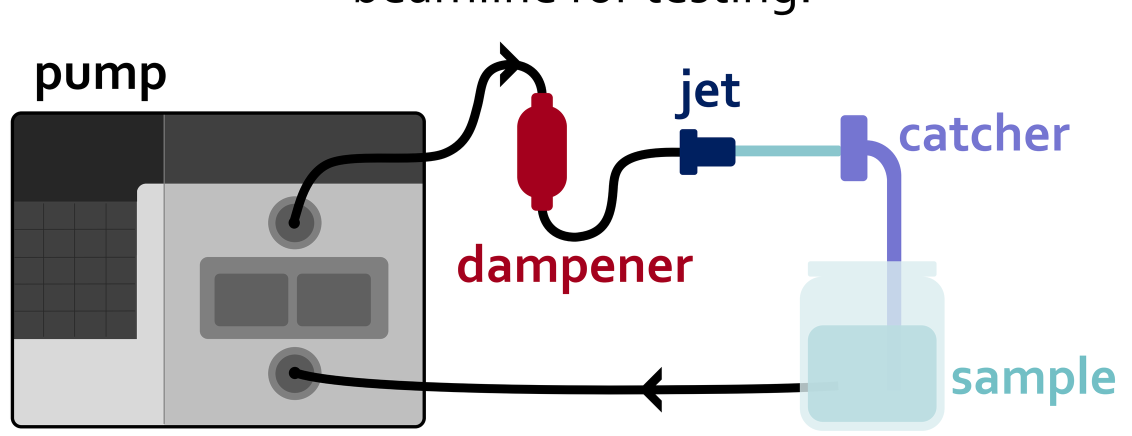

Figure 1: Jet testing setup. A double-plunger pump delivers sample to the jet at a specified flow rate and corresponding pressure. Jet stability fluctuates in time with each plunger stroke. Additionally, air bubbles erroneously brought into the pump from the sample reservoir exacerbate jet instability, and the plungers wind up striking against an air buffer. A hollow cylinder called a dampener is placed in the pump path to stabilize the jet. An air bubble forms at the top of the dampener, creating a buffer against the pump strokes and catching any bubbles that may have entered the pump tubing.

PRELIMINARY TESTING: CYLINDRICAL vs. SHEET

Cylindrical Jet

A cylindrical jet is formed by pumping liquid through a capillary. The inner diameter of the capillary will be the diameter of the jet.

Cylindrical jets flow relatively small volumes of liquid at relatively high pressures. The resulting liquid stream has a visible region of laminar flow before it becomes turbulent. In an experiment, the FEL pulses would strike in the laminar region.

Capillary diameter (µm)	50	75	100
Flow rate range (mL/min)	0.5 - 3	2 - 5	2 - 5
Pressure range (psi)	95 - 717	110 - 360	43 - 139
Laminar region range (mm)	2.25 – 3.15	5.73 -10.24	6.12 – 11.83

Table 1: Pump settings were changed to maximize laminar region

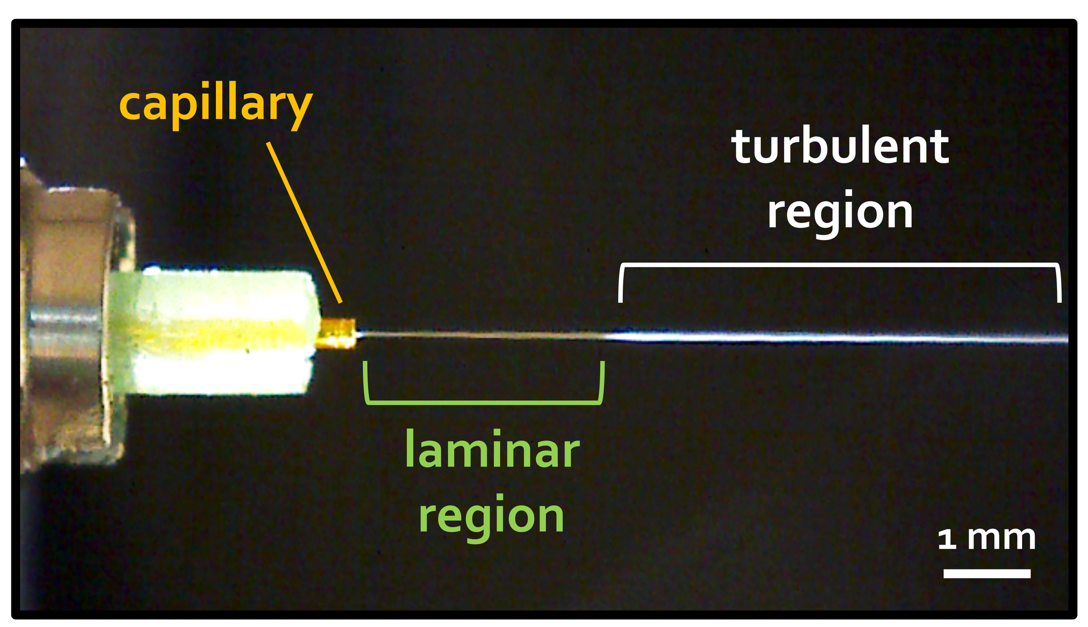

Figure 2: Cylindrical jet formed from a 50 µm diameter capillary running pure water at 0.8 mL/min and 160 psi.

Sheet Jet

Liquid is pumped through a glass chip that forms two streams and collides them, creating a series of sheets with decreasing size and alternating orthogonality. Thinness decreases nonlinearly over its length, but the total thickness range remains constant for a single chip nozzle size. Compared to the cylindrical jets, sheet jets flow much higher volumes of liquid at similar pressures.

Chip nozzle width (µm)	390	487	623
Flow rate range (mL/min)	15 - 30	15 - 30	15 - 35
Pressure range (psi)	103 - 210	95 - 190	90 - 180
Sheet length range (mm)	3.9 – 13.2	3.2 - 12.3	2.4 - 10.6

Table 2: Pump settings were changed to maximize sheet size

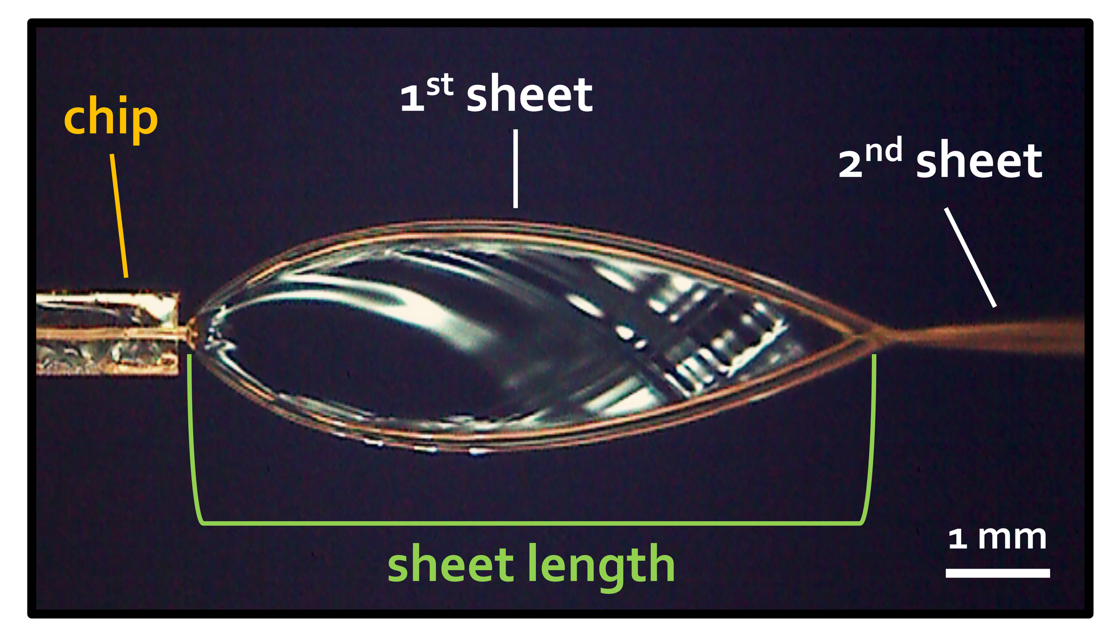

Figure 3: Sheet jet formed from a glass chip with 487 µm nozzle width running pure water at 25 mL/min and 144 psi.

CONCLUSIONS

Implications for Jet Choice

The preliminary data taken so far can already influence which jet a user may choose.

1. **Available sample volume:** Whether the user has ample or extremely limited sample size will factor heavily into their choice of jet, as the cylindrical jet operates with flow rates on the order of single mL/min while the the sheet jet requires tens of mL/min.
2. **Desired jet thickness:** The cylindrical jet's constant thickness means the FEL beam need only be aligned in the vertical axis. The sheet, on the other hand, has varying thickness, meaning the FEL beam must be precisely aligned in both the vertical and horizontal axes.
3. **Desired signal strength and snapshot precision:** The detected signal will increase as the respective FEL pulse intensity and jet thickness increase. However, a thinner jet can produce a more precise image of the sample, as less of the sample is being hit by the same intense pulse. The thinness of a cylindrical jet limits the pulse intensity, as the thinness also restricts the vertical space available to absorb the incoming pulse. The sheet, however, can maintain ample vertical space while producing an ultra-thin sample.

NEXT STEPS

Testing at the FEL

To most accurately build this guide, we must examine how each jet performs when exposed to the FEL.

1. We will vary the FEL pulse spot size to determine the intensity at which the pulse completely disrupts the jet flow.
2. We will vary the solvent used in the jet and monitor each solvent's evaporation rate under beam to determine the rate at which it should be replenished.

Ultimately, we would like to compile jet performance data to create a guide for LCLS users. A user would provide their sample information and desired jet thickness and beam conditions, and, by referencing the guide, we could easily direct them to the optimal jet and pump settings.

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