# Mail-In Fixed-Target SFX Chip Design and Handling Protocols

## -A Crystal Survival Guide

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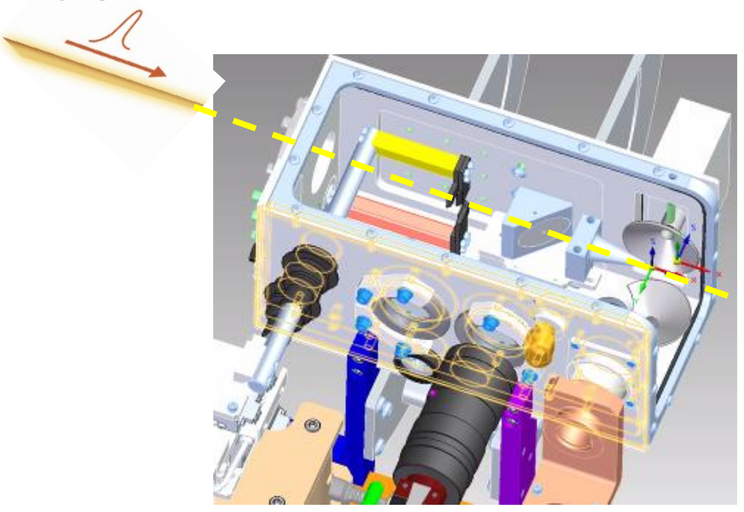
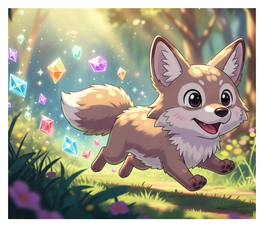
LCLS XFEL




**XFEL Crystallography Overview**
- X-ray Free Electron Laser creates diffraction patterns before crystals are destroyed.

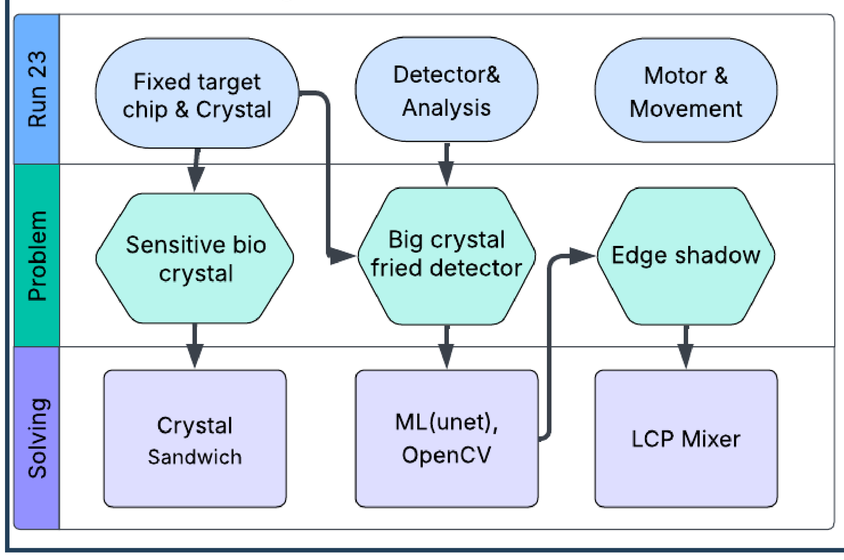
**Established Liquid Jet Methods & Disadvantages**
- Gas Dynamic Virtual Nozzle (GDVN), Electrospinning / MESH injectors, Drop-on-demand systems.
- Viscous liquids and larger crystals can clog or damage channels.
- Requires many crystals, with most never hit by the beam.

**Why & How Fixed Target Crystallography Works**
- Works well for scarce, fragile, or large crystals(in general).
- Crystals are loaded into patterned wells or on thin film.
- Chip is mounted in the beam path and scanned in a controlled sequence.
- Majority of crystals are exposed to the XFEL beam, collecting diffraction data from individual crystals.
- Main drawback: chip film has background scattering that reduce data quality.



Contact me if you are interested for more

## Project overview



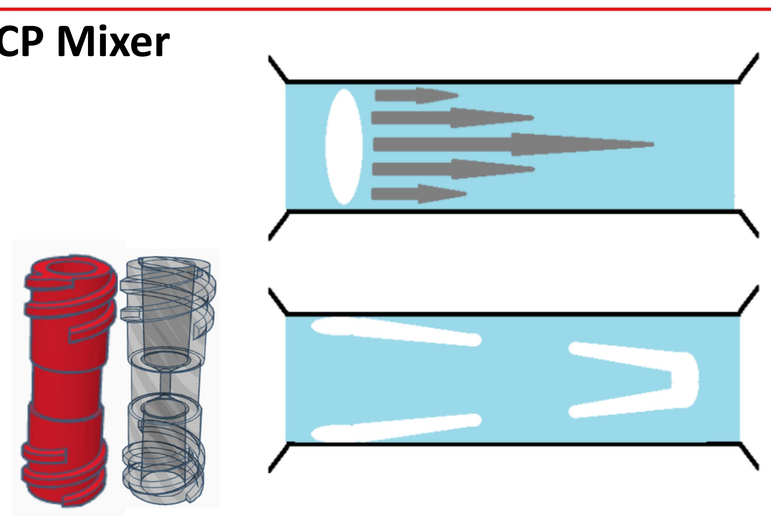

During Run 23 small-molecule crystallography at MFX, the ePix10k-2M detector was damaged by strong diffraction from large crystals, and some biocrystals degraded during preparation of the chip.

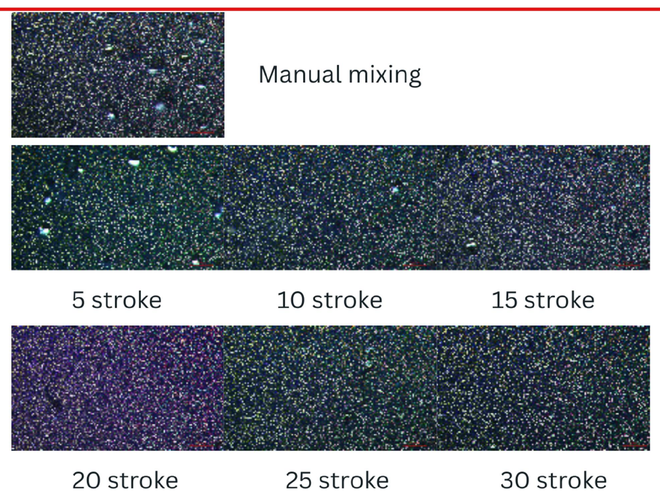
I began with a U-Net ML approach for image analysis, but it struggled to ignore dark bubble edges, so I moved to a more flexible OpenCV-based pipeline, which is still in progress.

I also tested a DIY LCP mixer to shear bubbles, reducing them to 10–20 µm so they can be skipped during image detection.

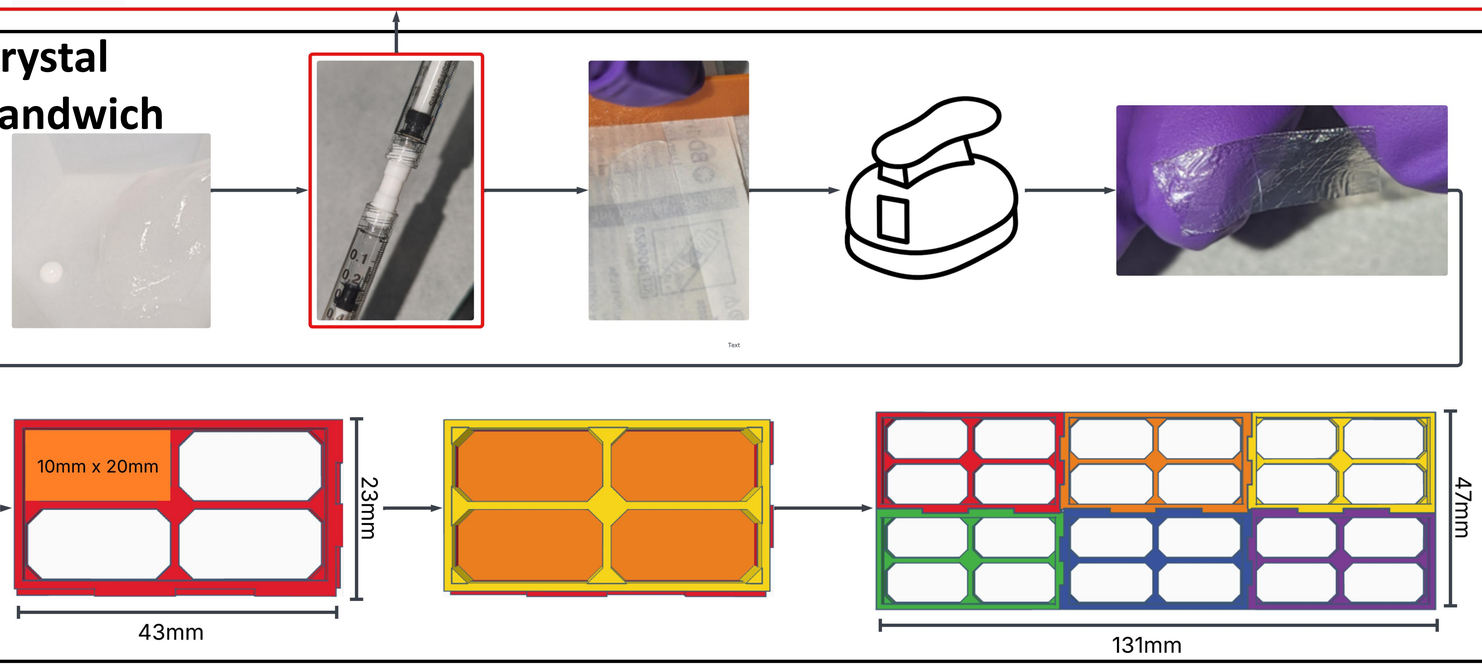
For chip design, I used a paper punch to cut grease–sample matrix sandwiches between 3 µm films and mounted them into a custom puzzle frame that can be reassembled after users prepare and mail in their chip sections.

## LCP Mixer



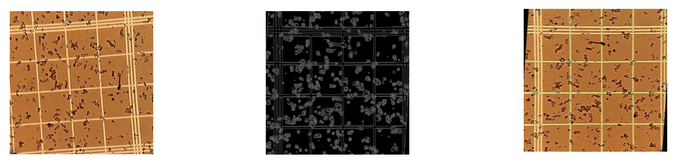



## Crystal Sandwich

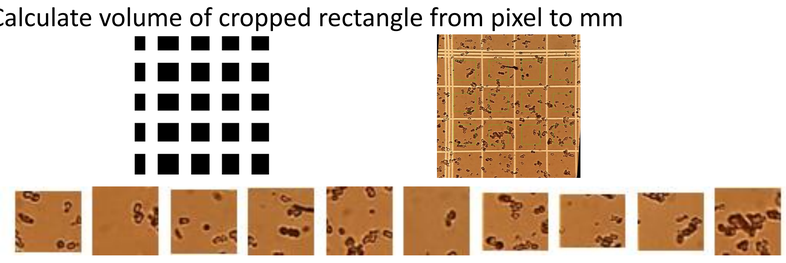



## OpenCV Method

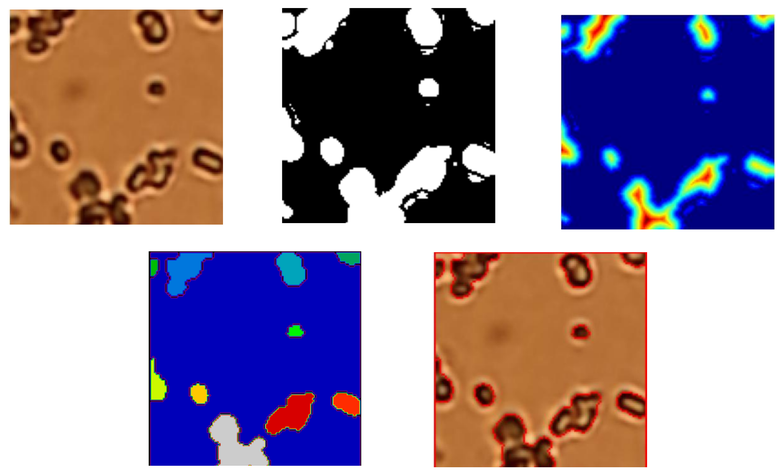
1. Rotate image (Canny edge, HoughLinesP),
2. Calculate pixel to mm by grid distance



3. Mask & Crop (Grid line masking)
4. Calculate volume of cropped rectangle from pixel to mm

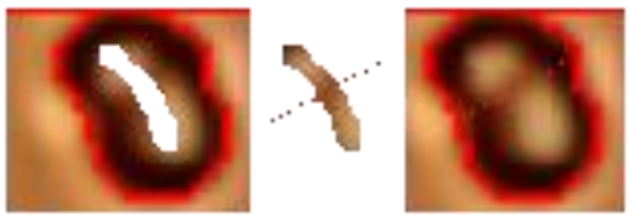


5. Outline Detection (Morphological Erosion + Distance Transform)



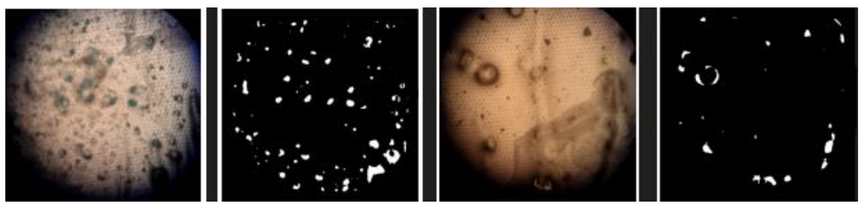
WORK IN PROGRESS

6. Backbone-Based Segmentation (Contrast Profiling Along Skeleton)



7. Data analysis. Count/volume, size distribution…

## Machine Learning (UNet) Method



References: Schriber, E.A., Paley, D.W., Bolotovsky, R. *et al.* Chemical crystallography by serial femtosecond X-ray diffraction. *Nature* **601**, 360–365 (2022).
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