Simulated X-ray Diffraction and Machine Learning for Interpretation of Dynamic Compression Experiments

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MSRF

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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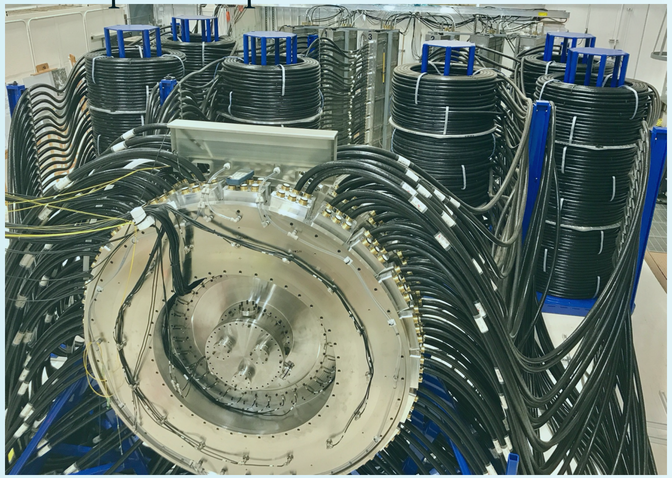
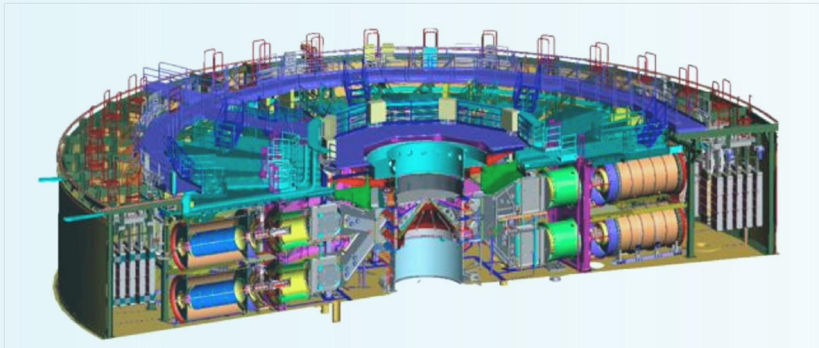
Dynamic compression experiment analysis using XRD: understanding the behavior of materials in extreme environments.

Thor and Z are pulsed-power accelerators which can drive shockless ramp waves to **pressures of 10s and 100s of GPa, respectively.**

Thor pulsed-power driver



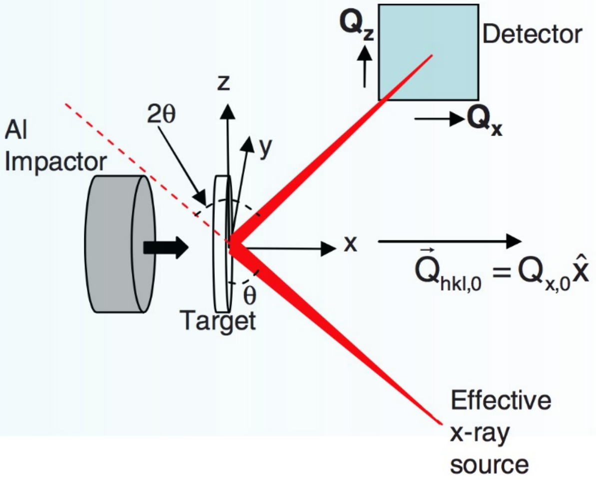
Z-machine at Sandia National Labs



33 m in diameter, 3 stories tall

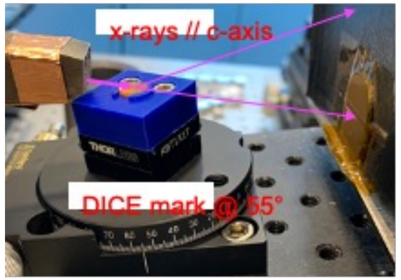
22 MJ stored energy
25 MA peak current
100-600 ns rise time

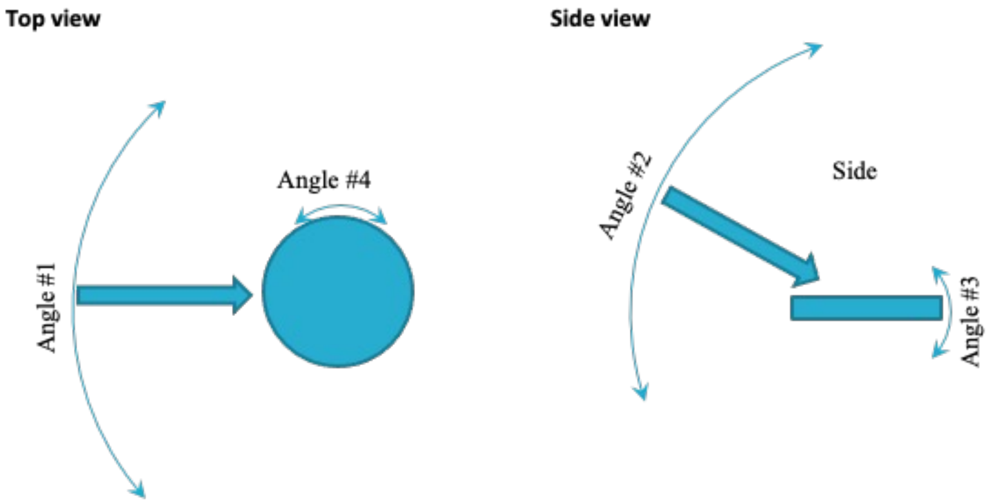
X-ray diffraction geometry



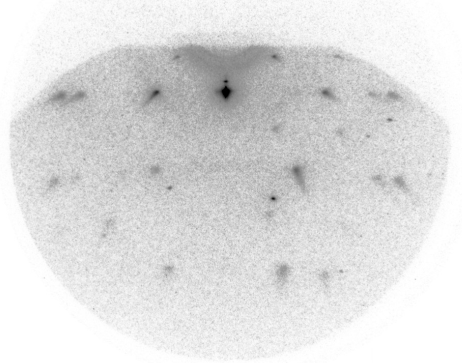
X-ray diffraction is key to deciphering the dynamic mechanisms and kinetics of phase transformation, because **it gives atomistic detail, structure & orientation**.

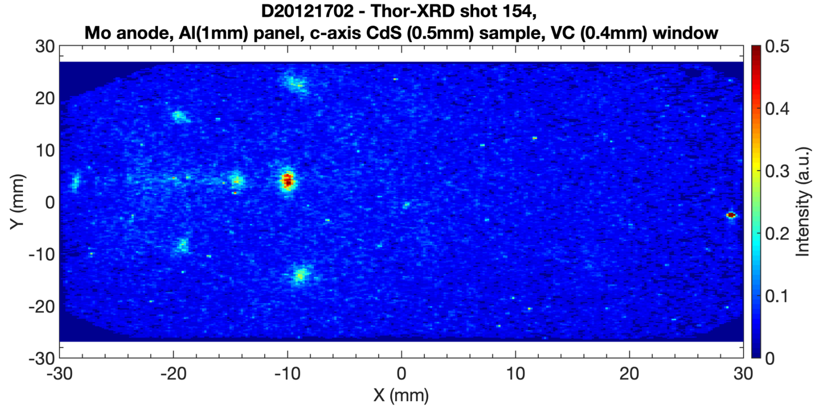
Dynamic compression experiment analysis using XRD: challenges associated with in-situ XRD

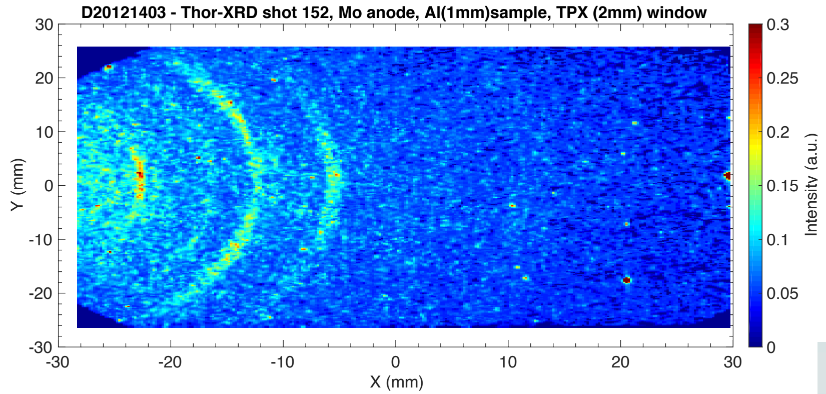




18-4-063 – DCS c-axis 1.683 km/s impact



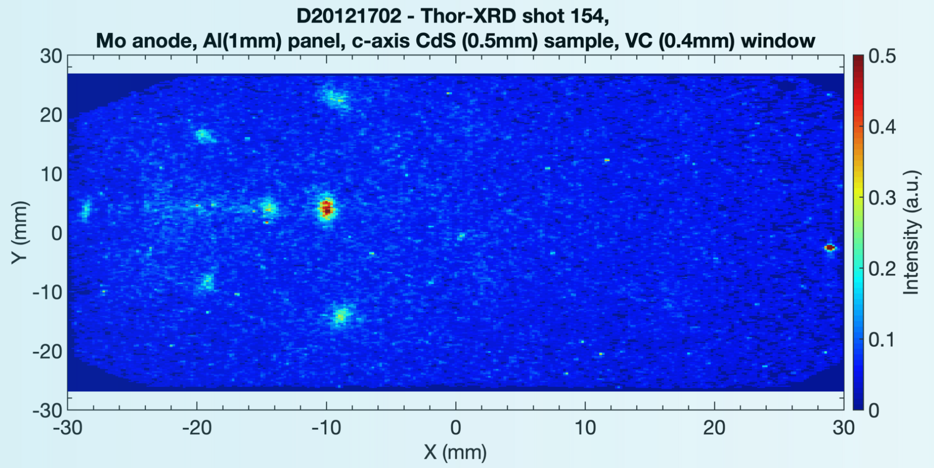


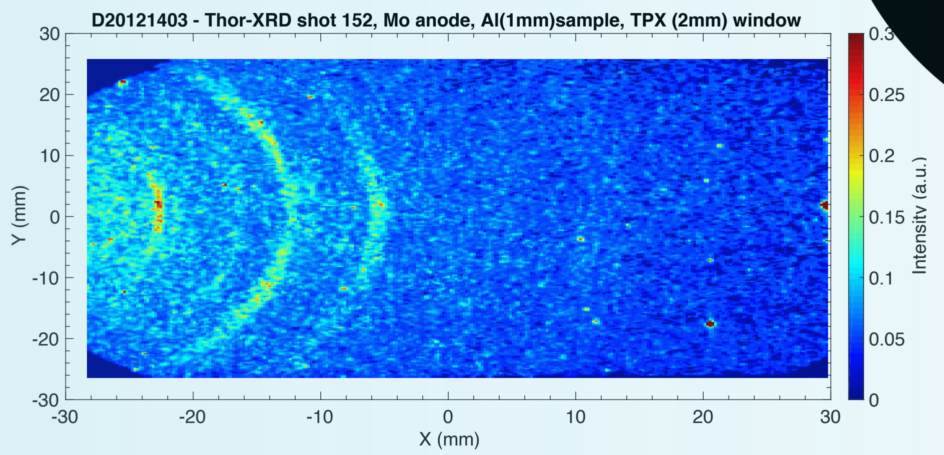


Analyzing XRD data is not trivial for many reasons:

- X-ray source can present collimation and has relatively broad spectra.
- The data obtained is sparse (one shot from Thor/Z generates one pattern).
- Noise is present in the obtained patterns from various sources (e.g., window, tamper, machine produced, etc.) .

Data-driven paradigm shift: optimizing interpretation of experimental XRD data .



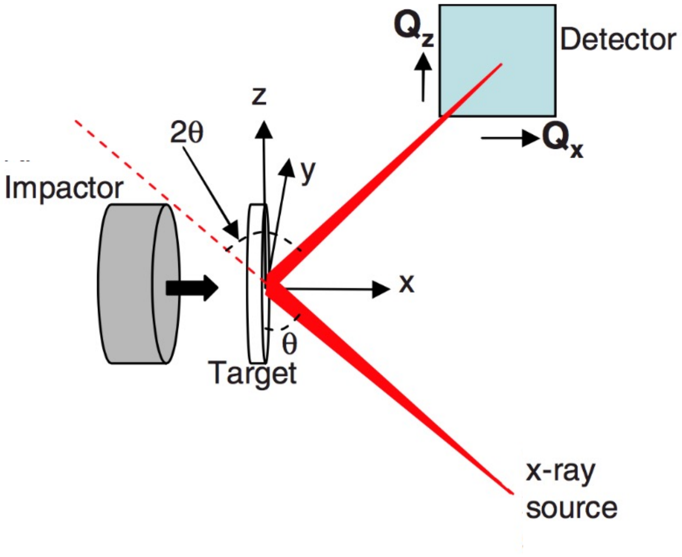


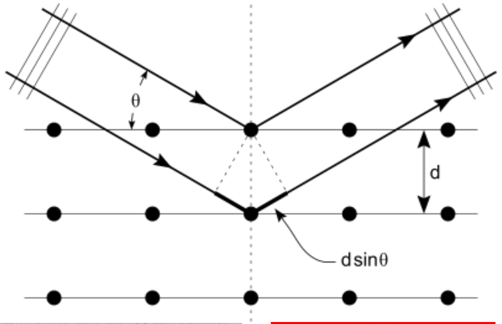
1) Orientation and lattice identification.

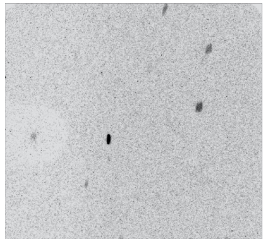
2) Denoising of Experimental Data.

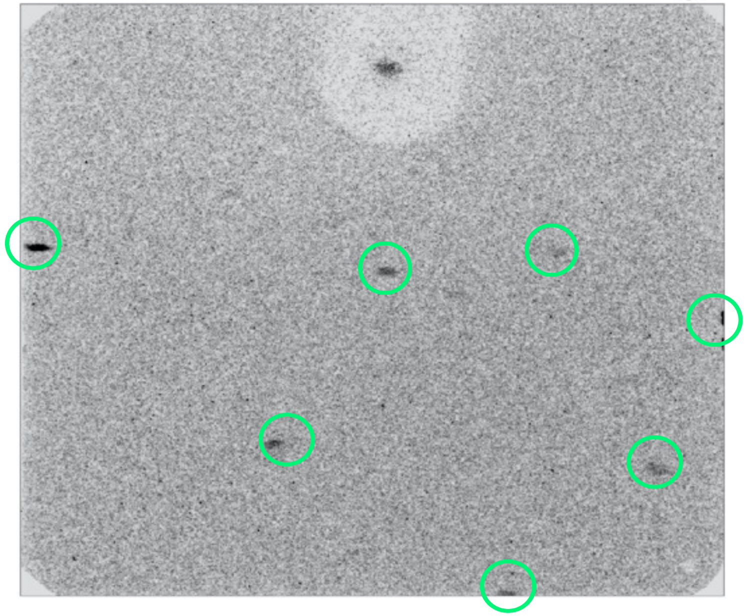
LAMMPS

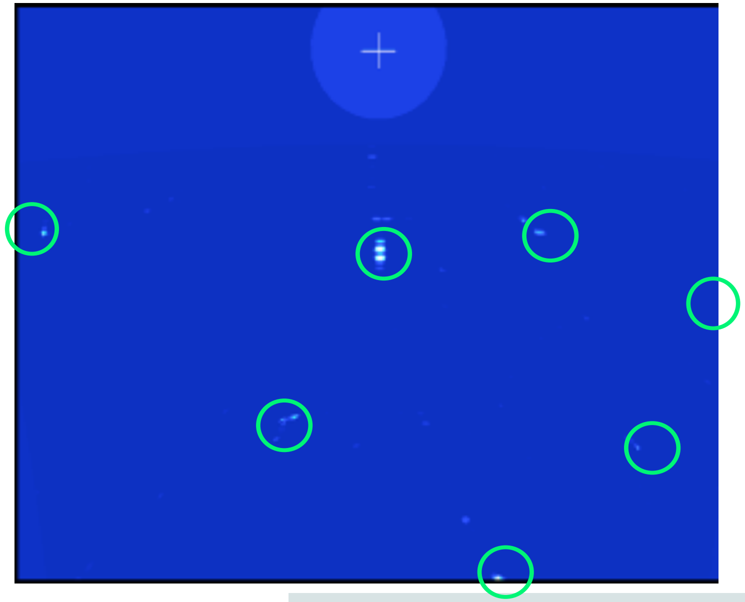
Simulated XRD: using LAMMPS to obtain realistic XRD patterns.







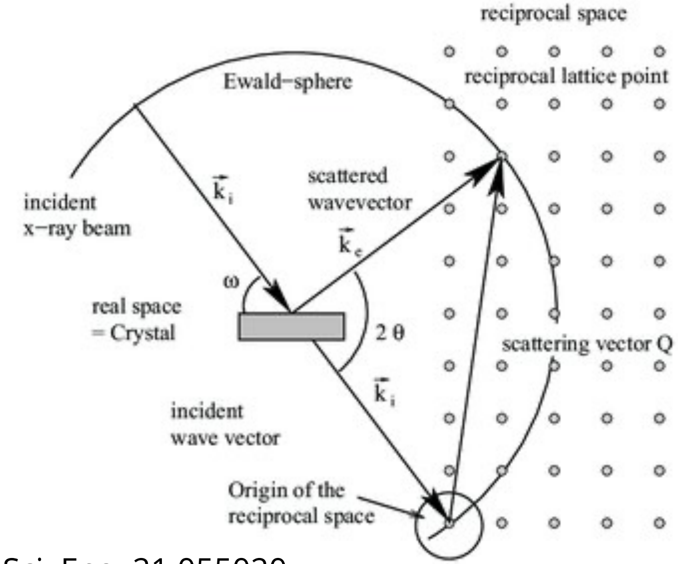




Constructing the Reciprocal space lattice in LAMMPS

$$F(\boldsymbol{K}) = \sum_{j=1}^{\#\text{atoms}} f_j(\theta) \exp\left(2\pi \mathrm{i} \boldsymbol{K} \cdot \boldsymbol{r}_j\right)$$

$$I_x(\boldsymbol{K}) = Lp(\theta) \frac{F(\boldsymbol{K})\, F^*(\boldsymbol{K})}{N}$$

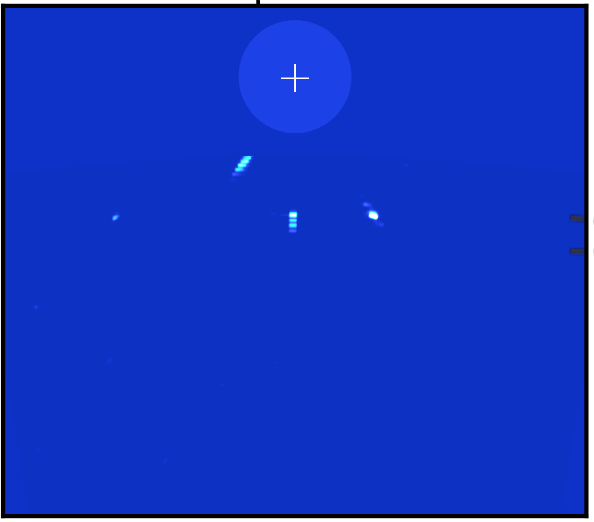


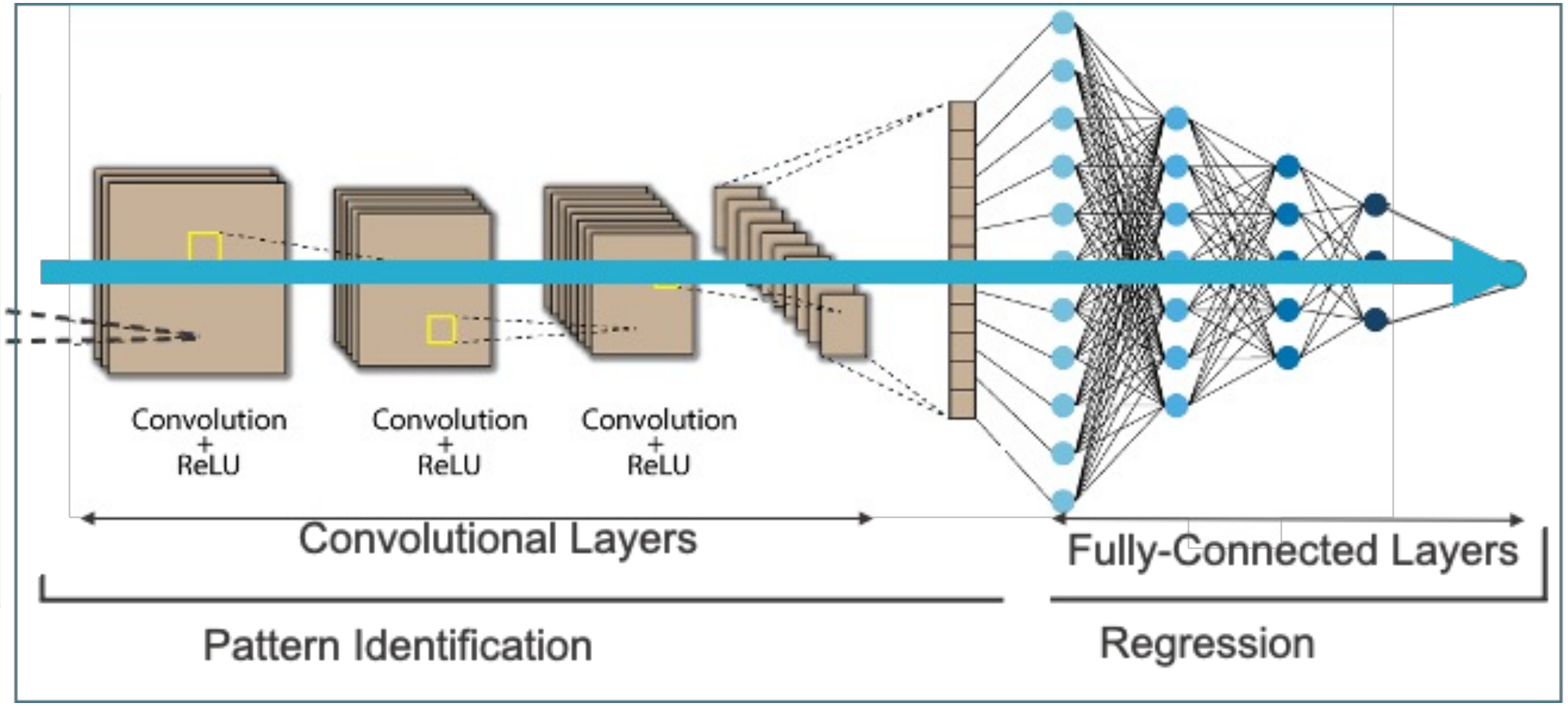
Lp(q) is the Lorentz-polarization factor
And f_j are the atomic scattering factors

Coleman et al., 2013 Modelling Simul. Mater. Sci. Eng. 21 055020

Data-Driven Analysis I: Determining the Crystal Lattice and Orientation Angle using Deep Learning (DL).

Input



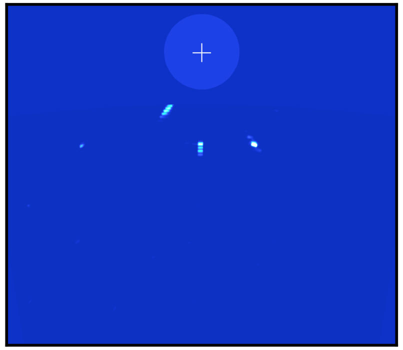


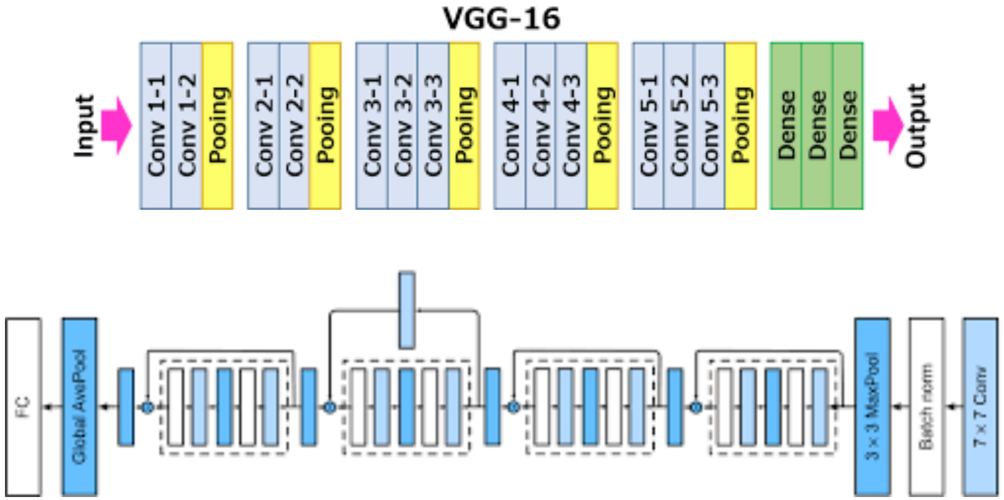
Output

Orientation Angle

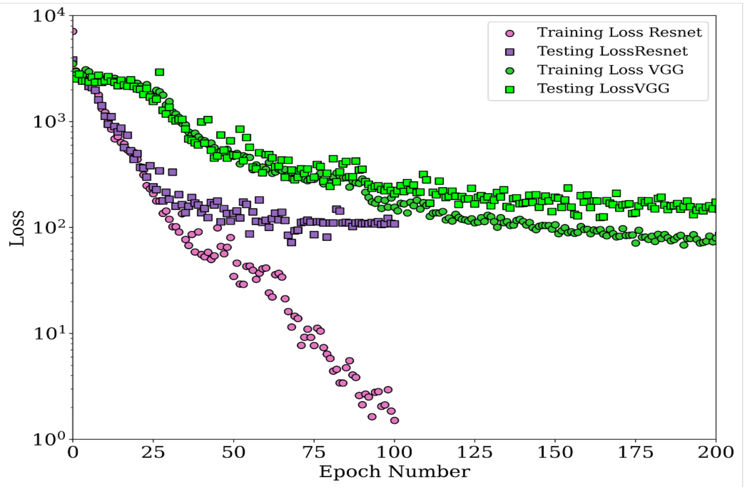
Data-Driven Analysis I: Incorporating Physics into the DL-based model.

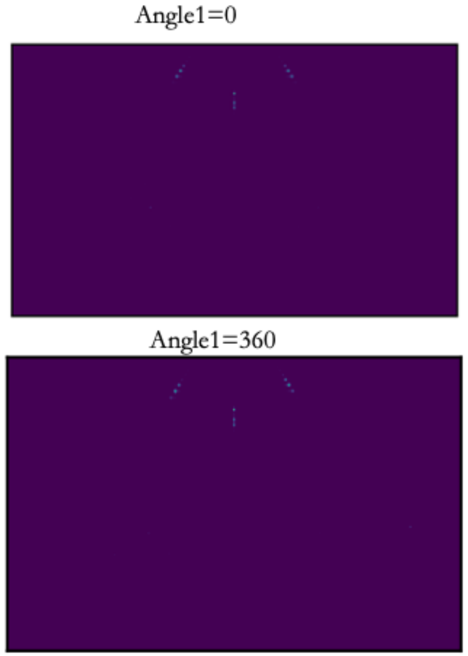
Input:
20k+ images – four angle



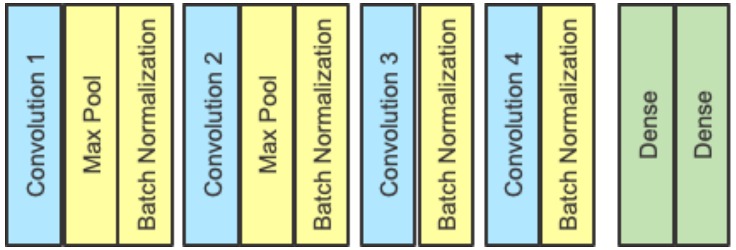


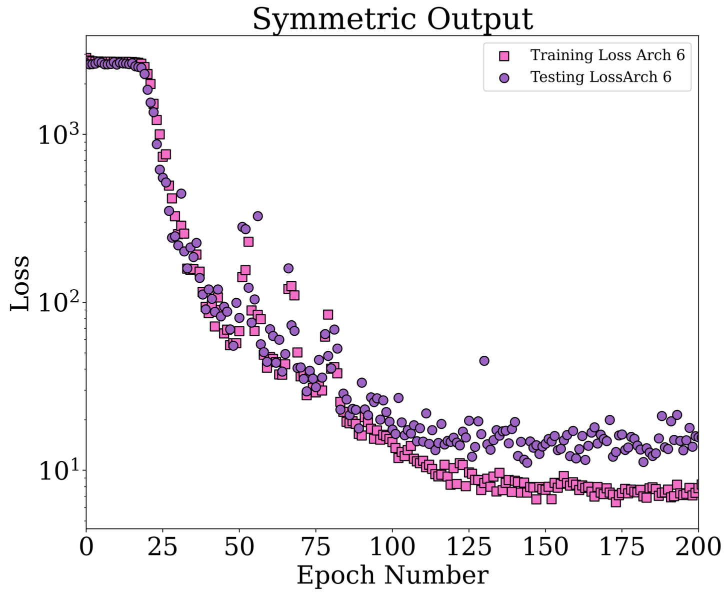
$$Loss = mean(angle_{predicted} - angle_{true})^2$$



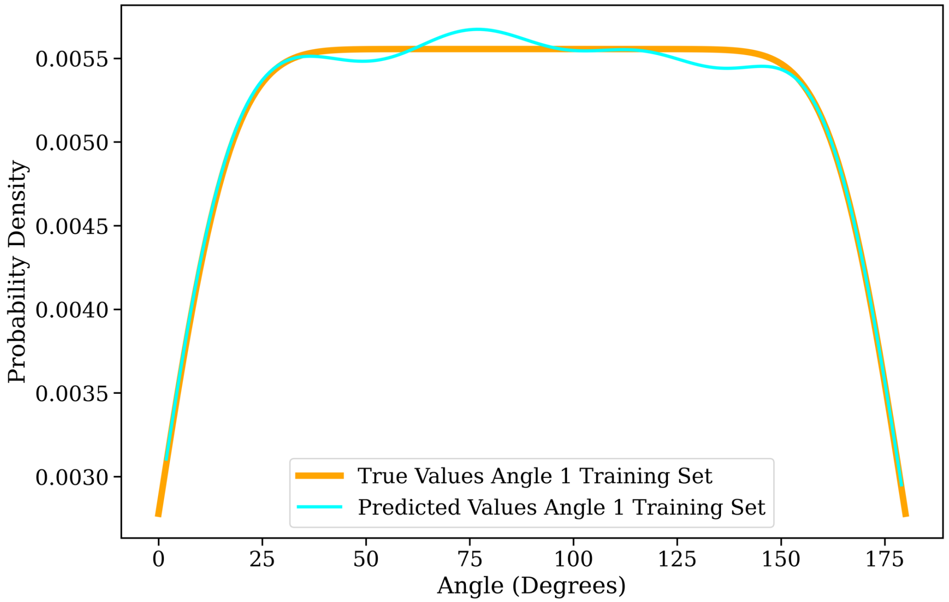


Input:
- 720 images – one angle
- Manually incorporate symmetry
- Constrain model to predict value between 0 and 180

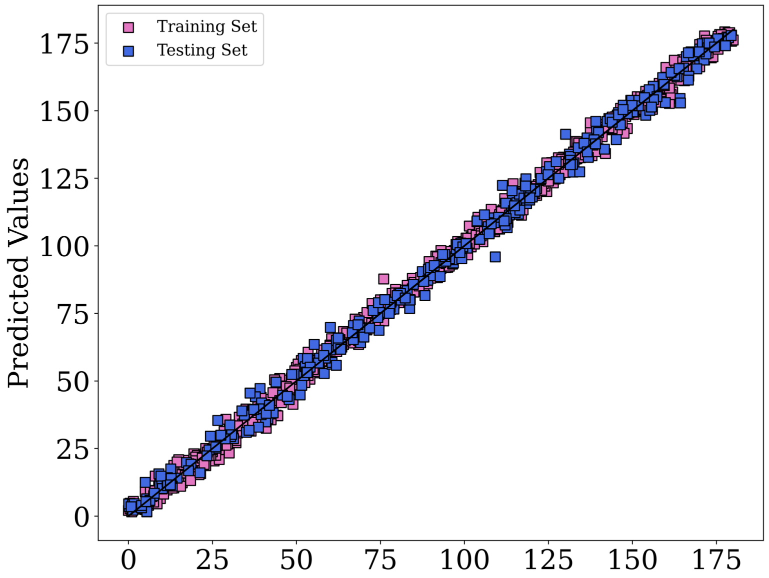




Data-Driven Analysis I: Results and next steps.

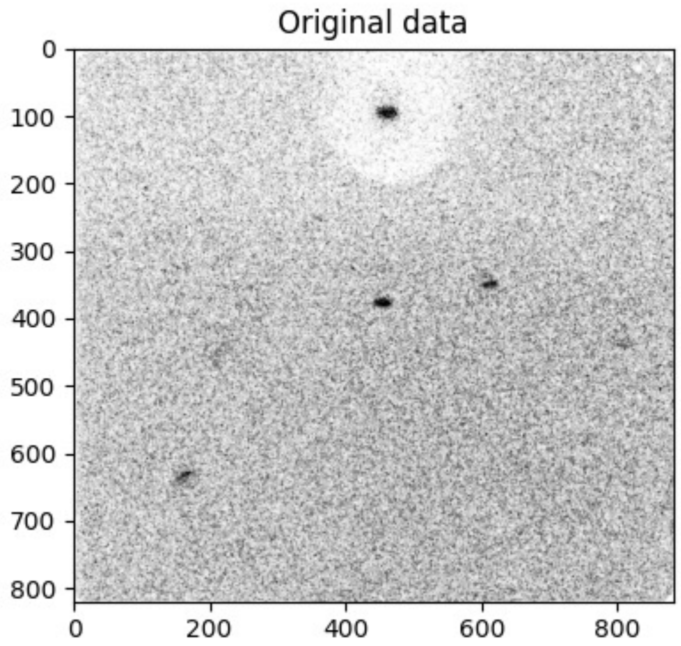


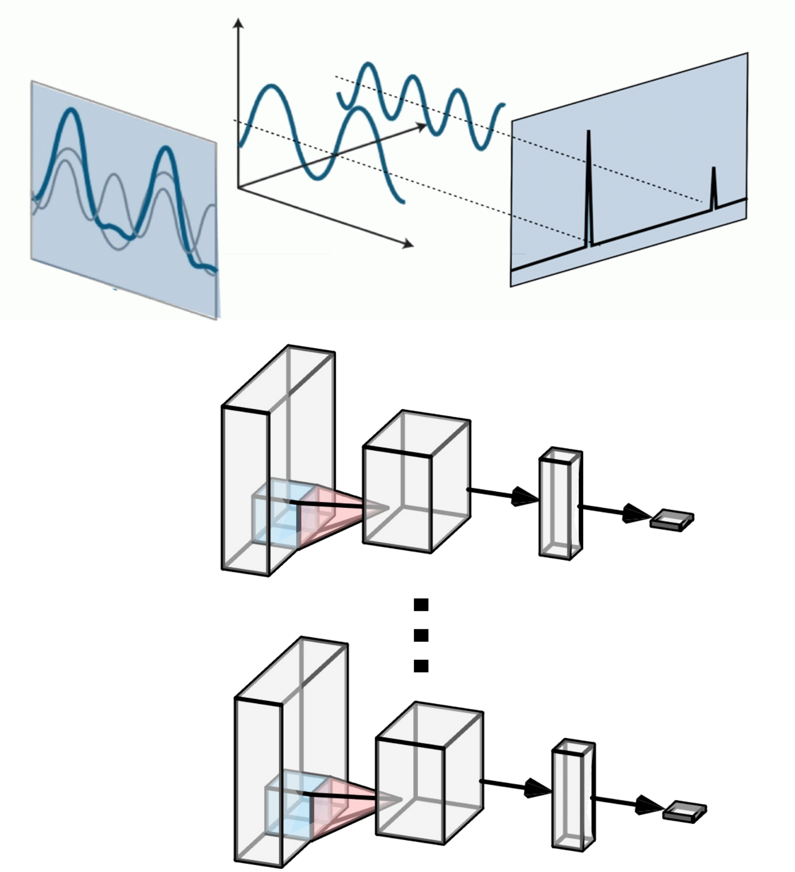
Test Set consists of 300 XRD patterns generated from angles between 0 and 360 on which the model has not been trained.

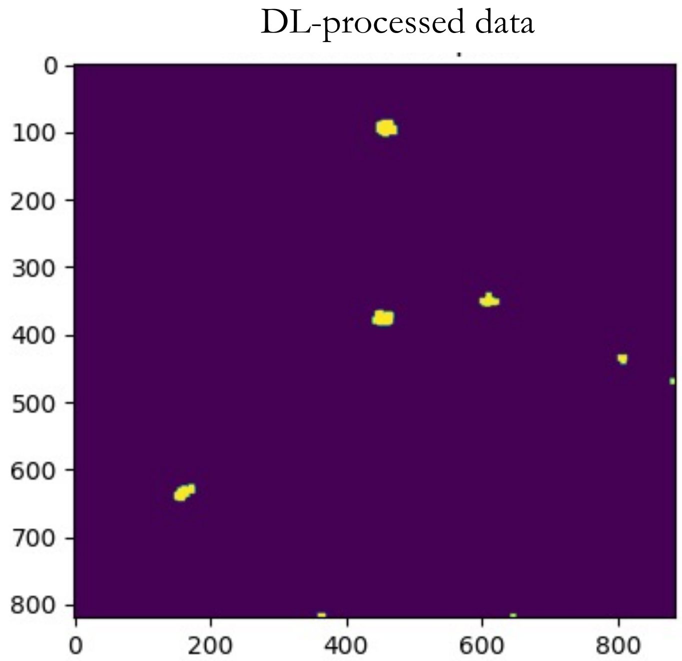


- Successful training of a single-angle ML tool is proof of concept, moving to two and four angle models present scaling challenges.
- Automate symmetry identification to reduce the data necessary.
- Using uncertainty as a our objective we can train an adaptive model that in an automatic way samples the regions of the input domain needed to establish a robust model with an optimal resolution.

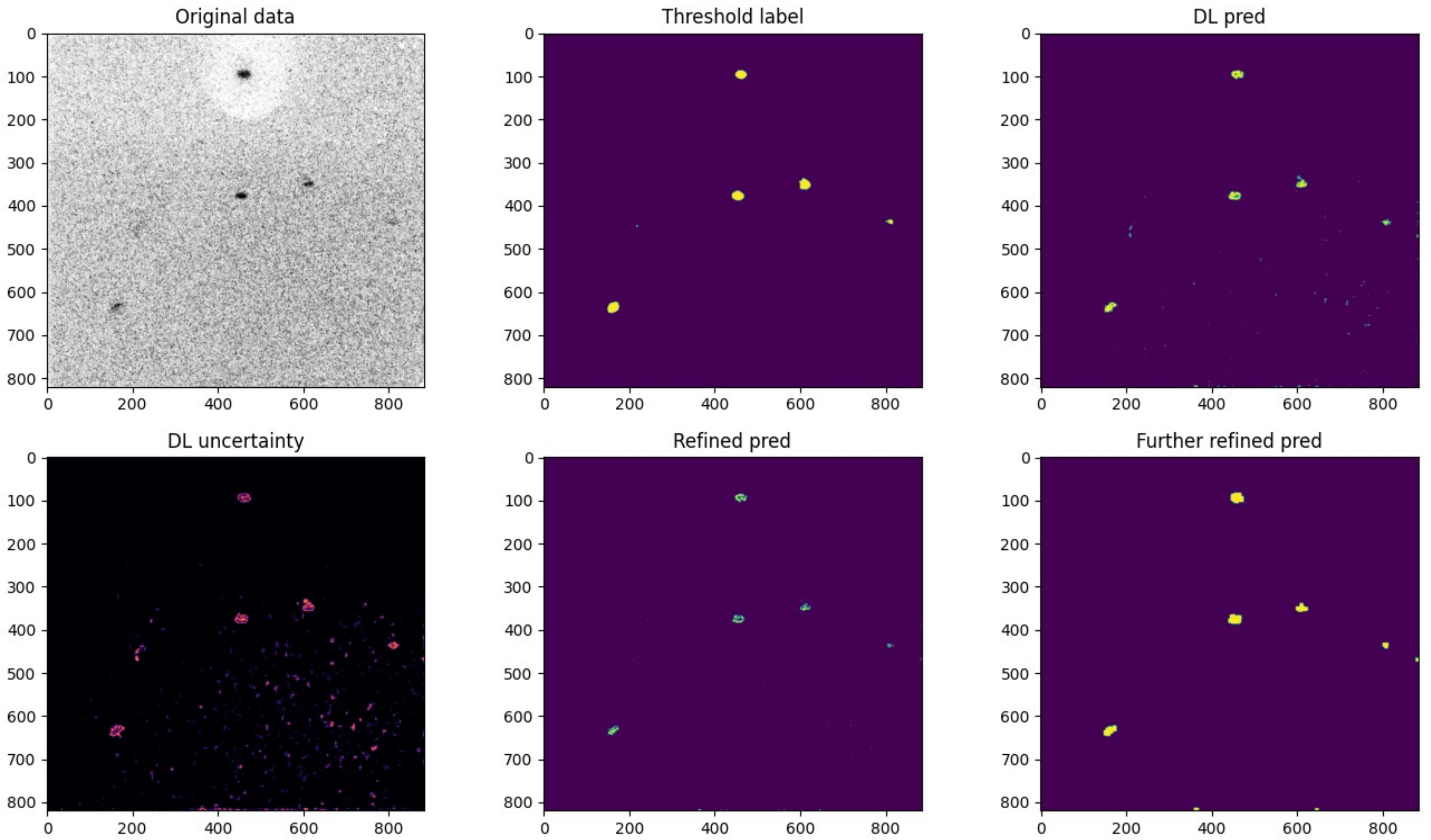
Data-Driven Analysis II: Removing experimental noise using Deep Learning.







Data-Driven Analysis II: DL-based de-noising protocol.



- U-Net architecture that predicts class of each pixel in input image.

Olaf Ronneberger, Philipp Fischer, Thomas Brox , "U-Net: Convolutional Networks for Biomedical Image Segmentation", in Medical Image Computing and Computer-Assisted Intervention (MICCAI), Springer, LNCS, Vol.9351: 234--241, 2015.

- **DL segmentation predictions provide per-pixel uncertainty estimates**. We remove noise from the prediction by removing pixels whose predictions were uncertain (bottom, center).

Martinez, C., et al. (2019). Segmentation certainty through uncertainty: Uncertainty-refined binary volumetric segmentation under multifactor domain shift. In Proceedings of the IEEE/CVF CVPRW.

- Gaps in the prediction are filled with standard image processing methods (bottom, right).

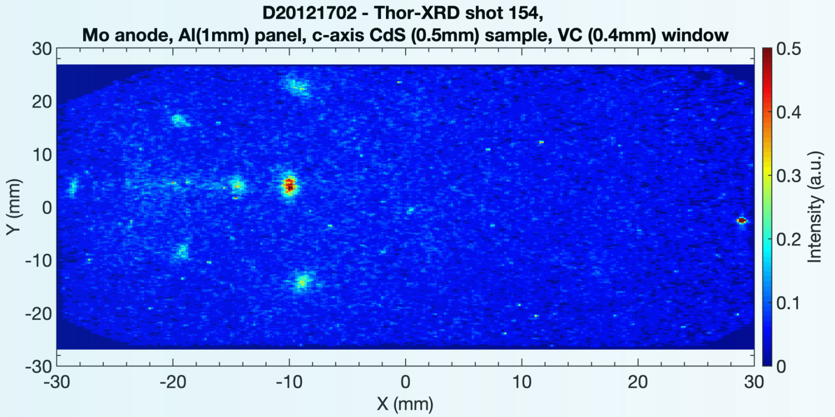
Deep learning algorithm learns to separate diffraction signal from noise given ~20 training examples with rough labels.

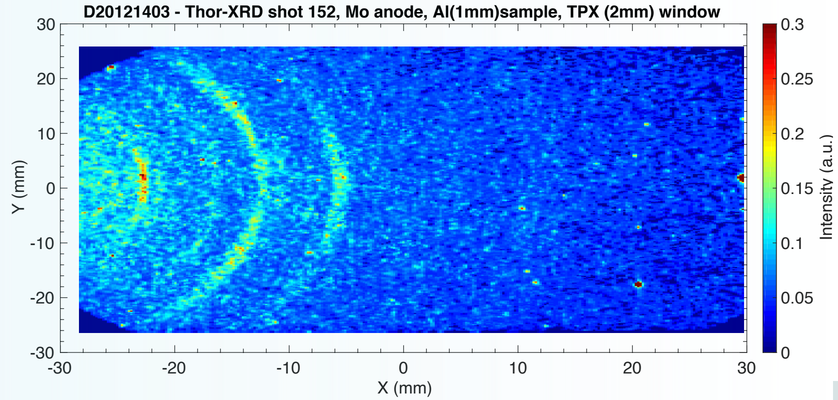
Conclusions: ML-enhanced interpretation of XRD patterns from dynamic compression experiments.

ML and computational data-driven techniques **enable the development of robust tools to enhance and better interpret dynamic X-ray diffraction data** produced from Sandia's Pulsed Power Platforms (Thor and Z).

The developed tools will **dramatically improve our atomic-scale understanding** and predictive capability of phase transition behavior.

Opens new research avenues by **enabling new state-of-the-art experiments** to probe phase transitions, microstructural evolution, and transformation mechanisms.





Questions?