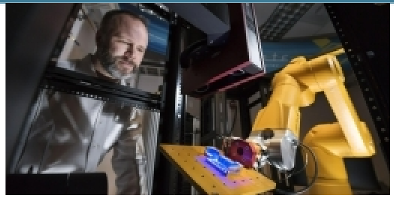
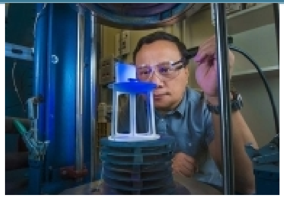
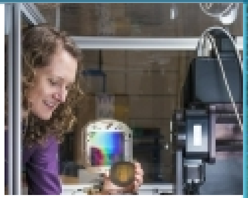
SAND2022-8913C

Sandia National Laboratories

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



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MSRF

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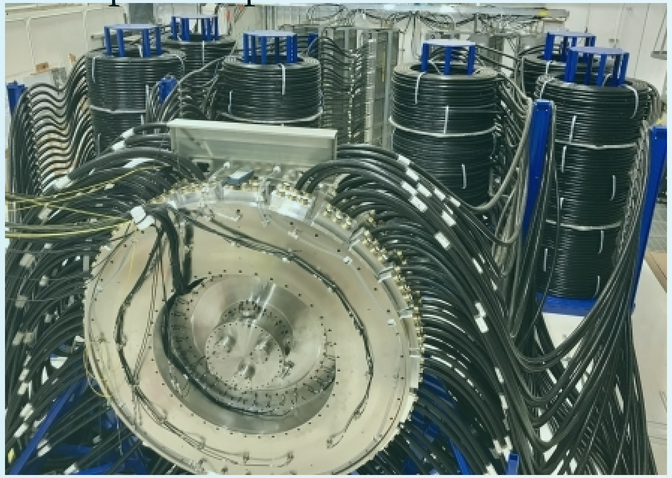
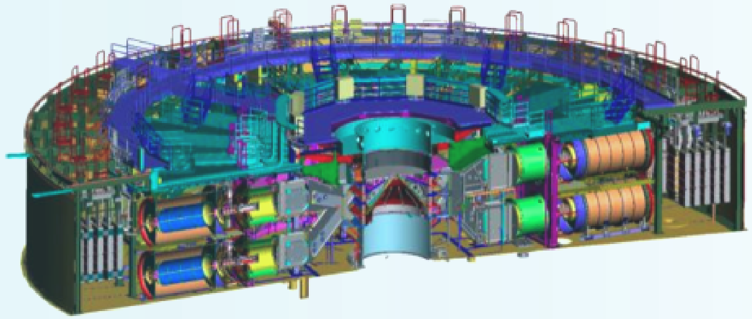
# Dynamic compression experiment analysis using XRD: understanding the behavior of materials in extreme environments.

**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



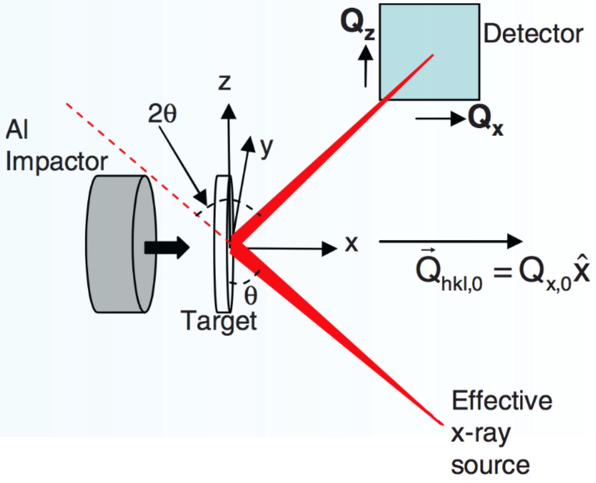
Z-machine at Sandia National Labs



33 m in diameter, 3 stories tall

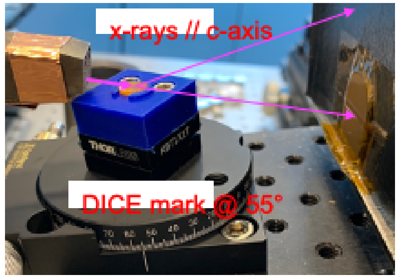
22 MJ stored energy
25 MA peak current
100-600 ns rise time

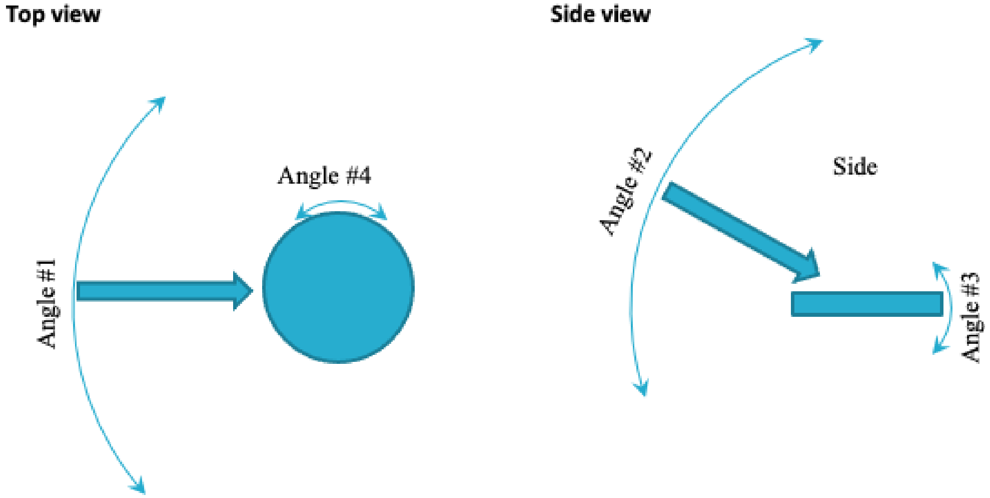
X-ray diffraction geometry



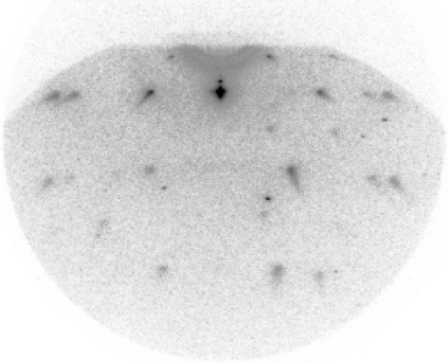

X-ray diffraction is key to deciphering the dynamic mechanisms and kinetics of phase transformation, because **it gives atomistic detail, structure & orientation**.

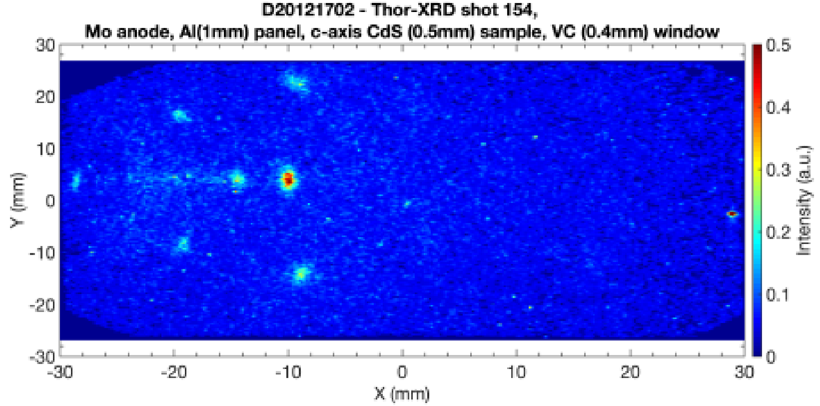
# Dynamic compression experiment analysis using XRD: challenges associated with in-situ XRD

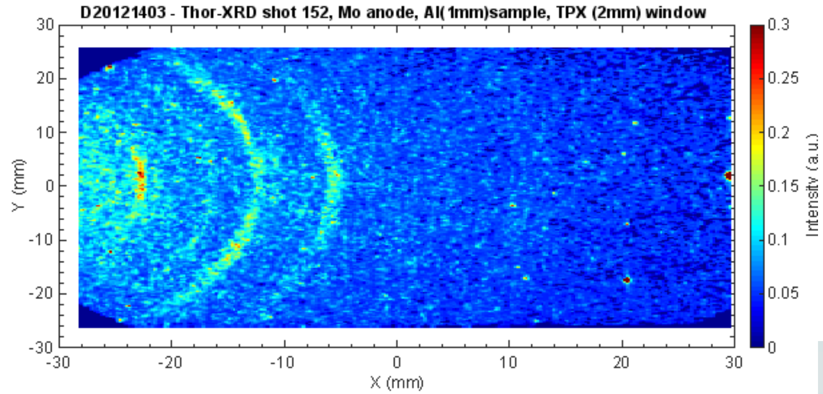



*18-4-063 – DCS c-axis 1.683 km/s impact*



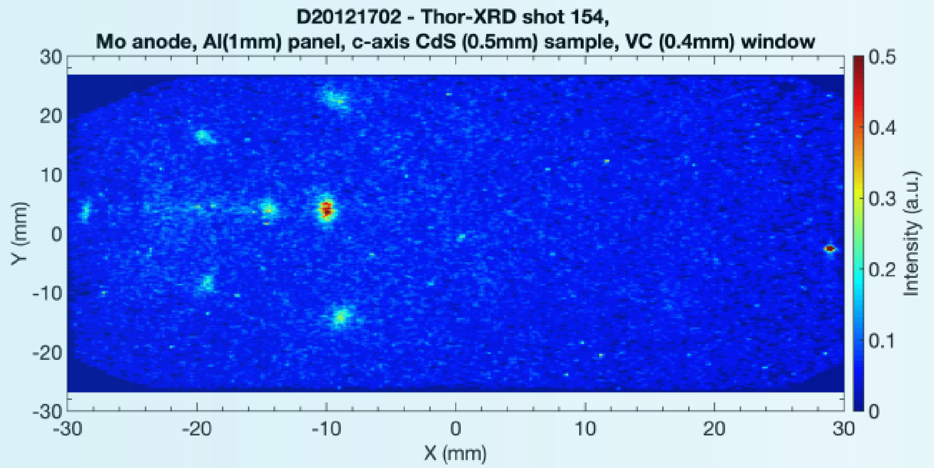


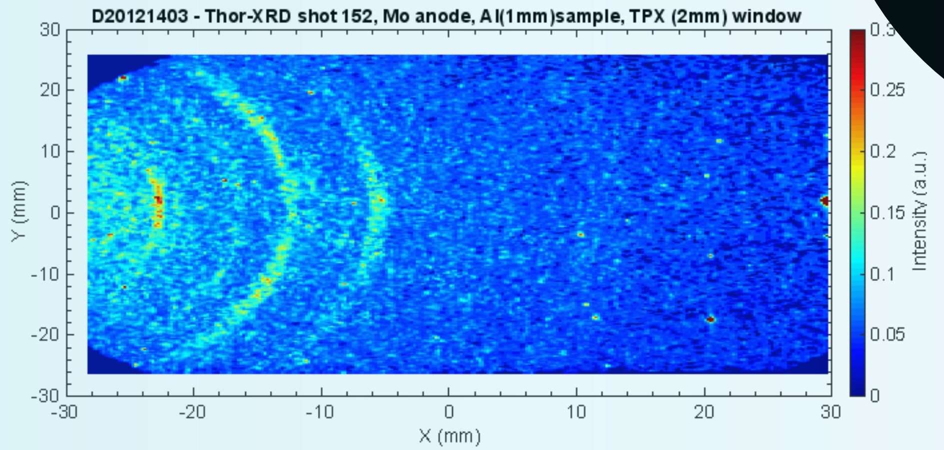



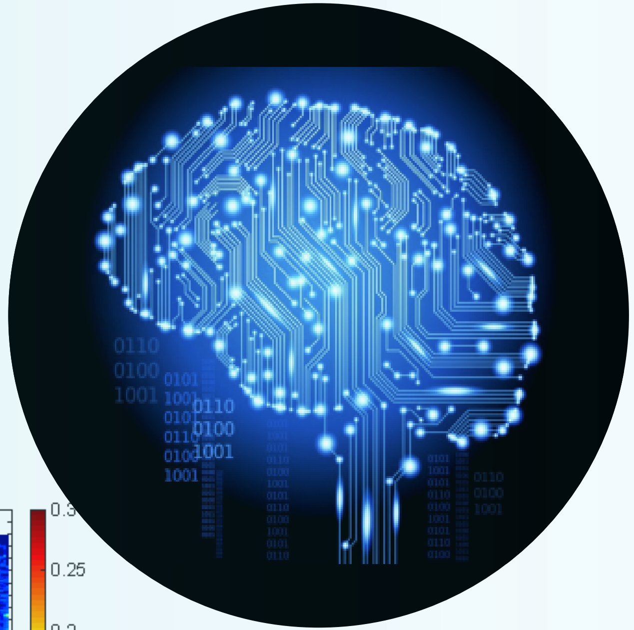

Analyzing XRD data is not trivial for many reasons:

- 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 .



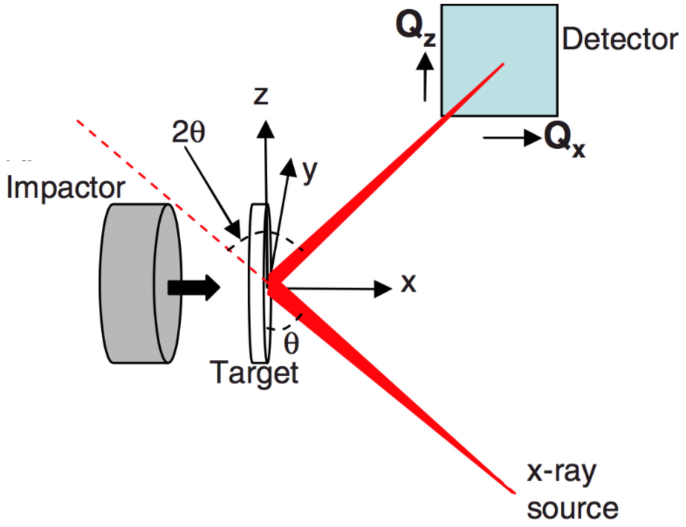



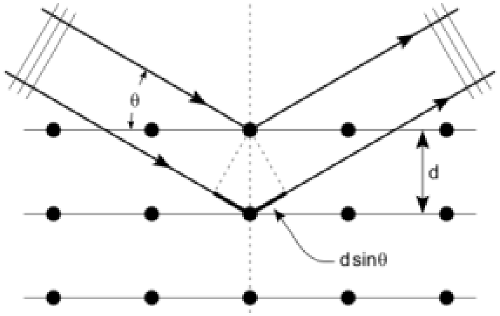



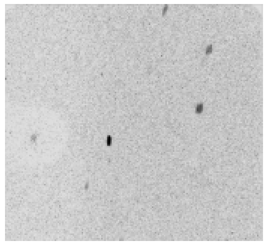
1) Orientation and lattice identification.

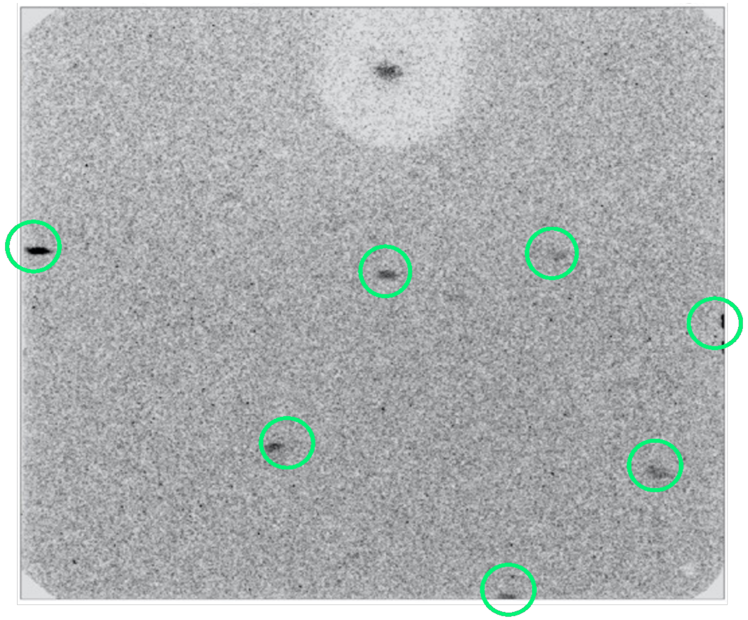
2) Denoising of Experimental Data.

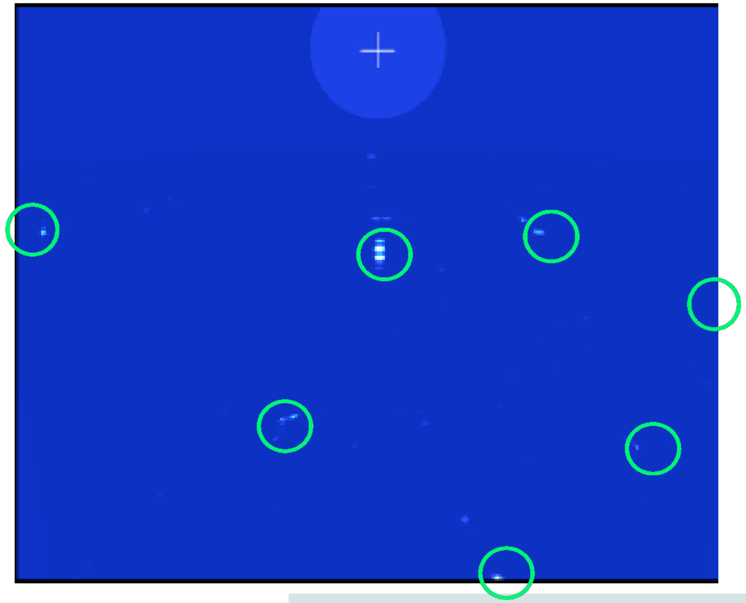
# **Simulated XRD:** using LAMMPS to obtain realistic XRD patterns.



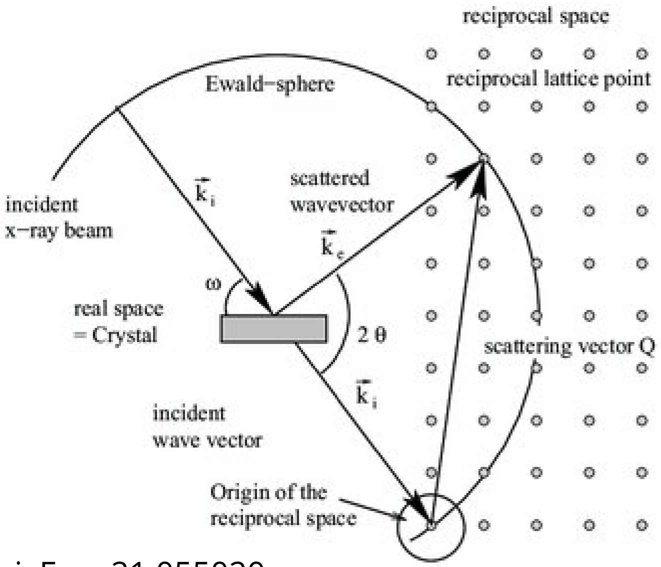




Constructing the Reciprocal space lattice in LAMMPS

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

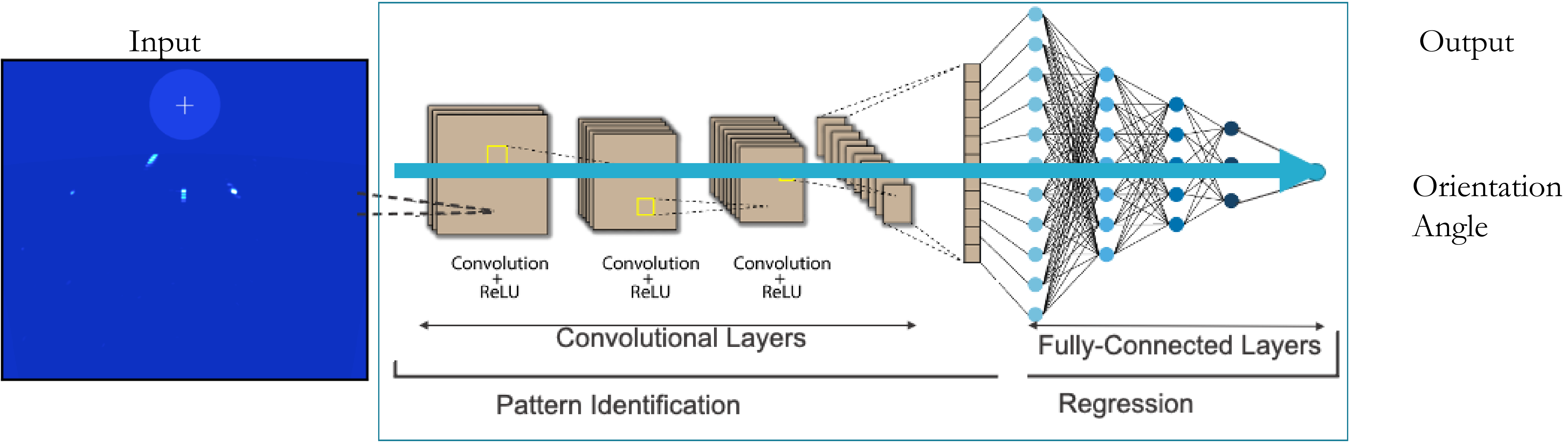
$$I_x(\boldsymbol{K}) = Lp(\theta) \frac{F(\boldsymbol{K}) F^*(\boldsymbol{K})}{N}$$




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

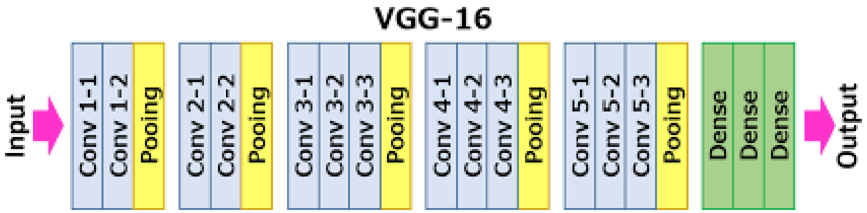
Coleman et al., 2013 Modelling Simul. Mater. Sci. Eng. 21 055020

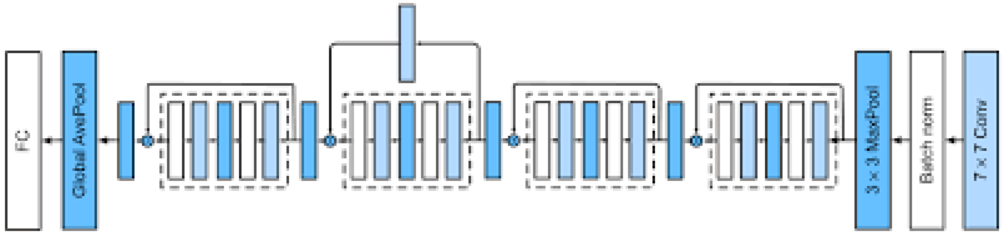
# Data-Driven Analysis I: Determining the Crystal Lattice and Orientation Angle using Deep Learning (DL).



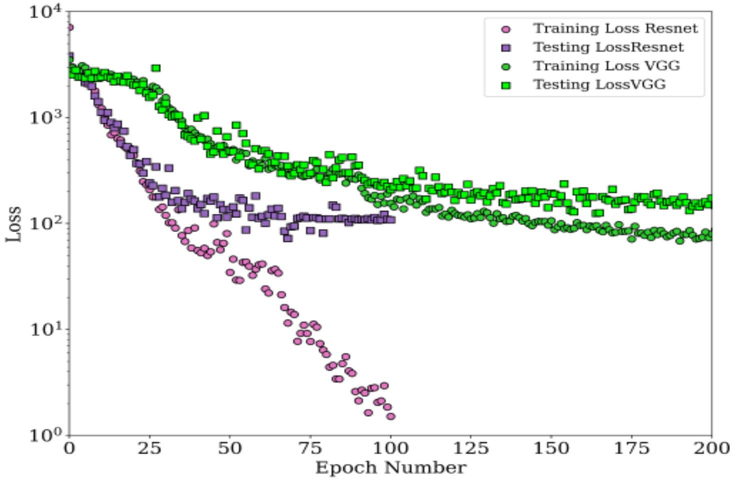
# Data-Driven Analysis I: Incorporating Physics into the DL-based model.

**Input:**
20k+ images – four angle




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

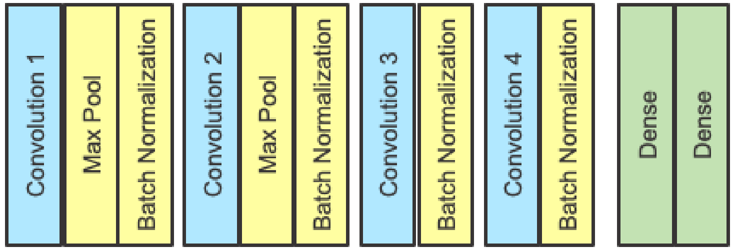


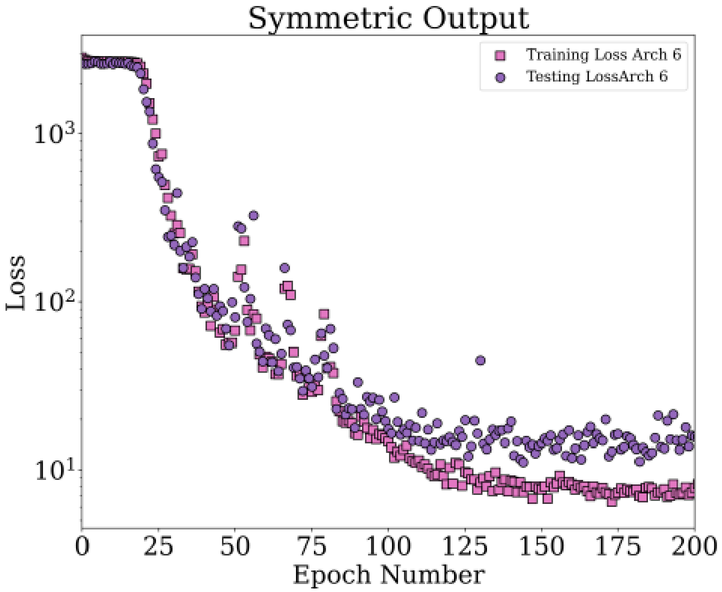

Angle1=0

Angle1=360

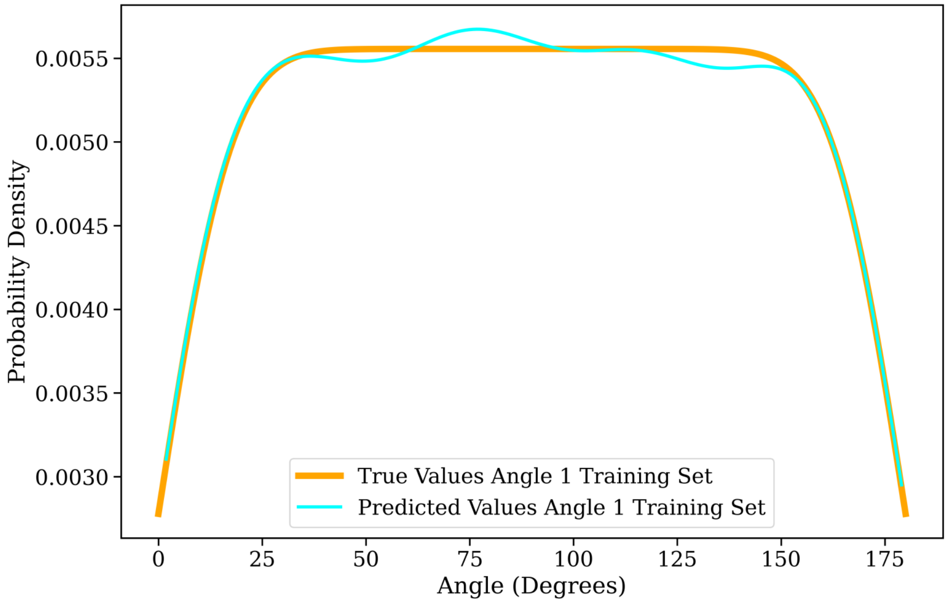
**Input:**

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



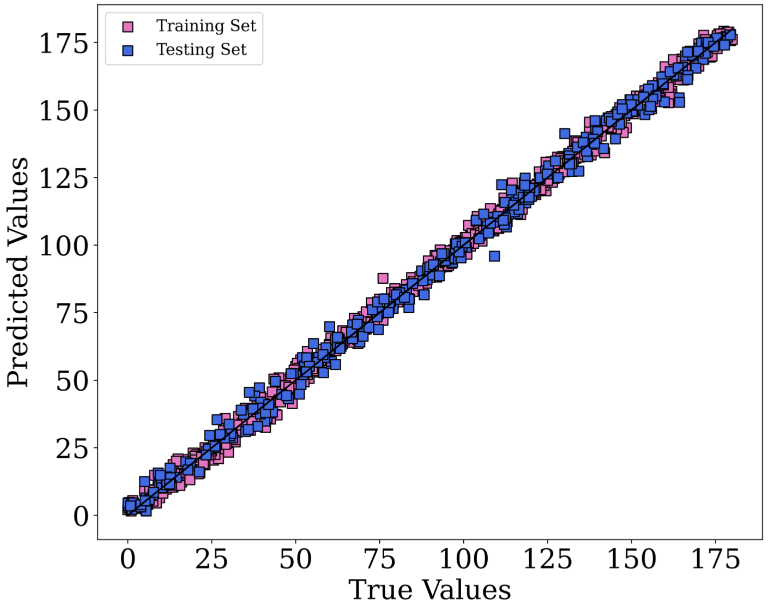



# Data-Driven Analysis I: Results and next steps.



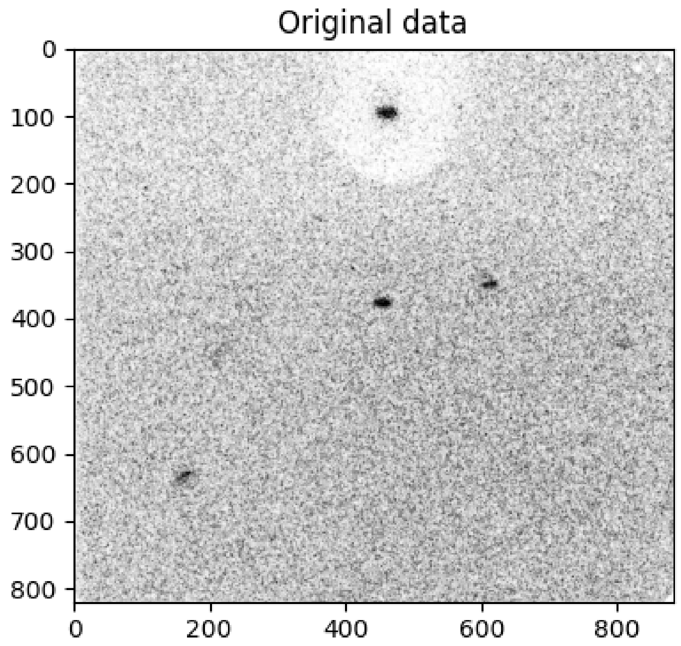


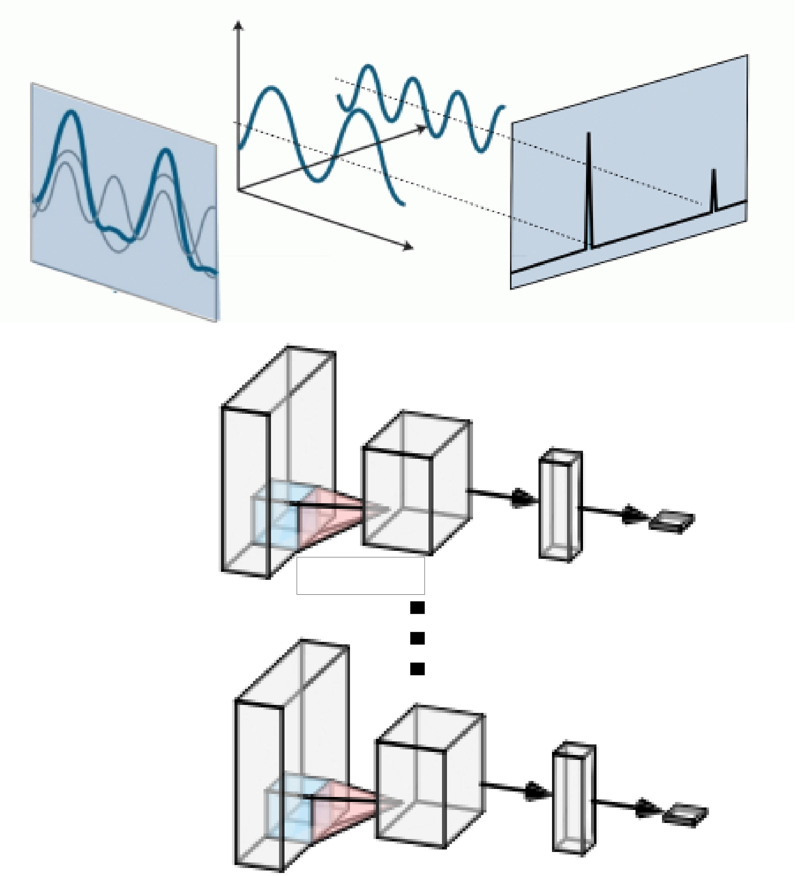
Test Set consists of 300 XRD patterns generated from angles between 0 and 360 on which the model has not been trained.

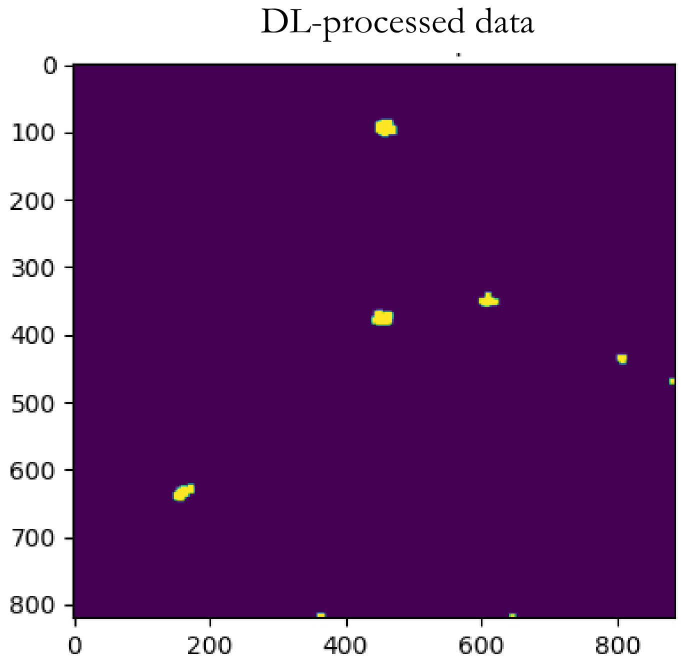



- Successful training of a single-angle ML tool is proof of concept, moving to two and four angle models present scaling challenges.
- Automate symmetry identification to reduce the data necessary.
- Using uncertainty as a our objective we can train an adaptive model that in an automatic way samples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

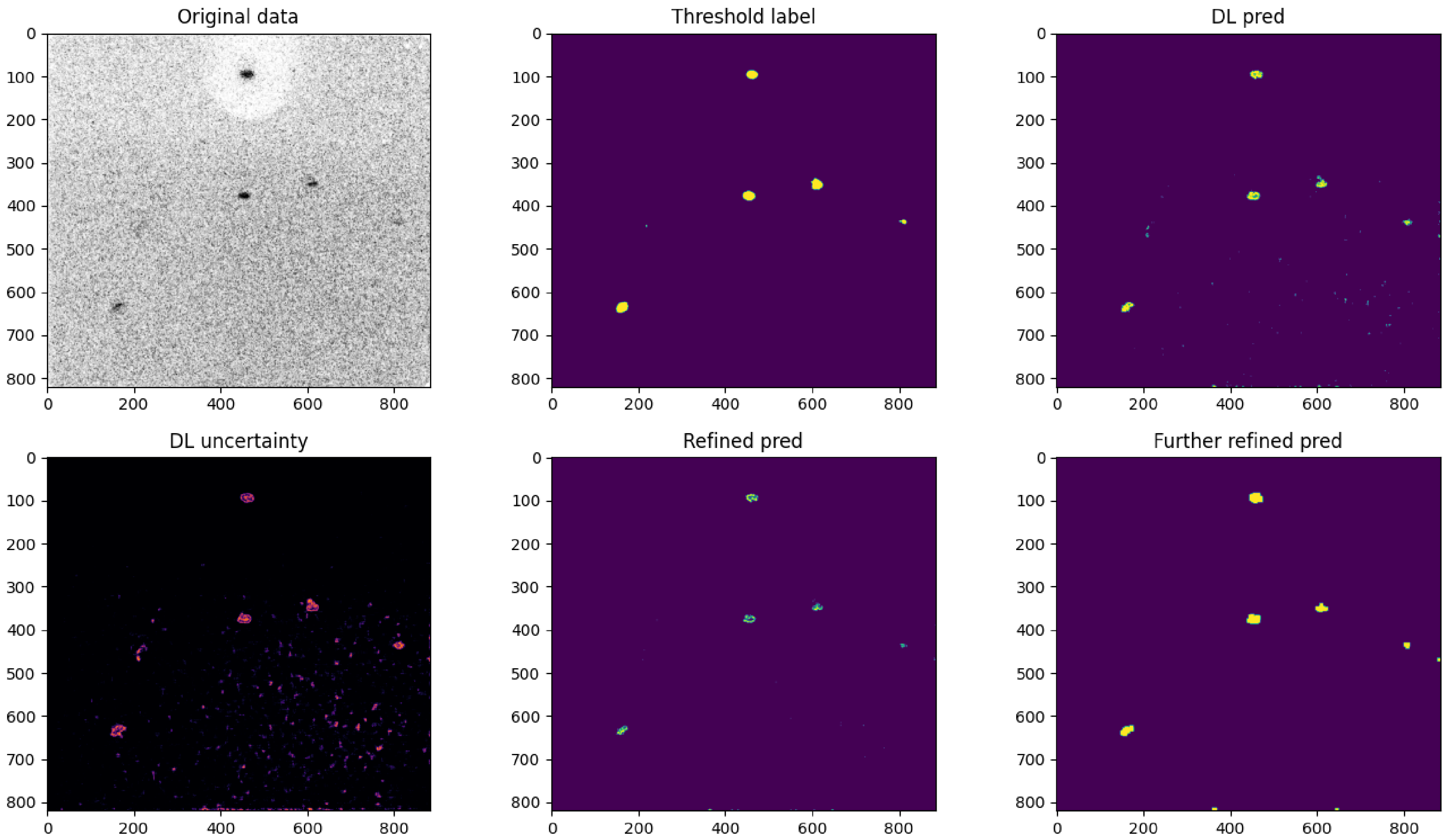
# Data-Driven Analysis II: Removing experimental noise using Deep Learning.





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




**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.

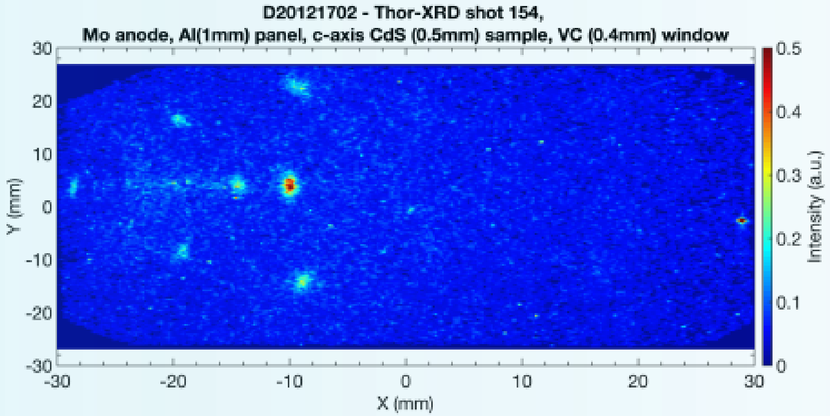
Gaps in the prediction are filled with standard image processing methods (bottom, right).

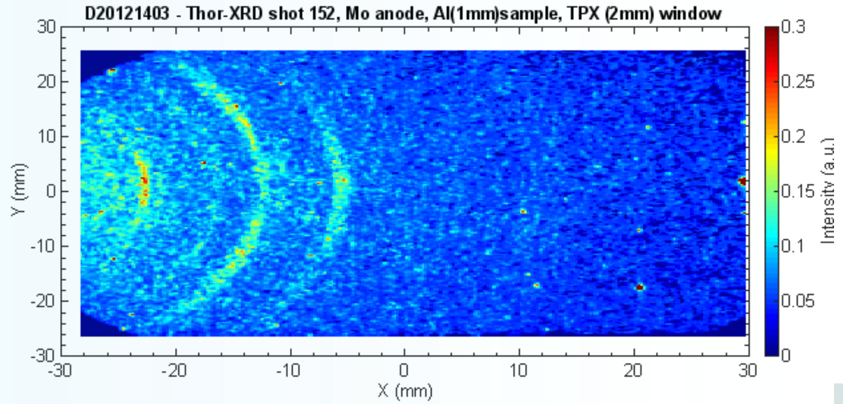
# **Conclusions:** ML-enhanced interpretation of XRD patterns from dynamic compression experiments.


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.

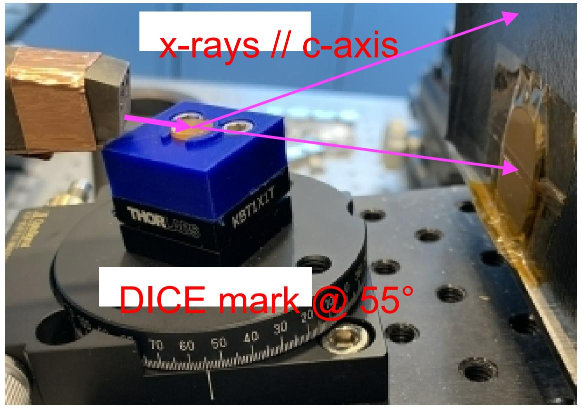
Opens new research avenues by **enabling new state-of-the-art experiments** to probe phase transitions, microstructural evolution, and transformation mechanisms.



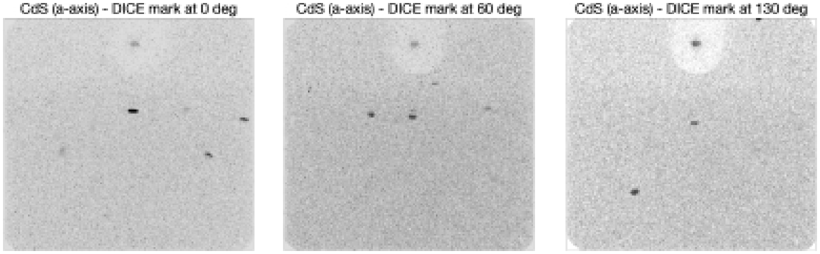
# Questions?

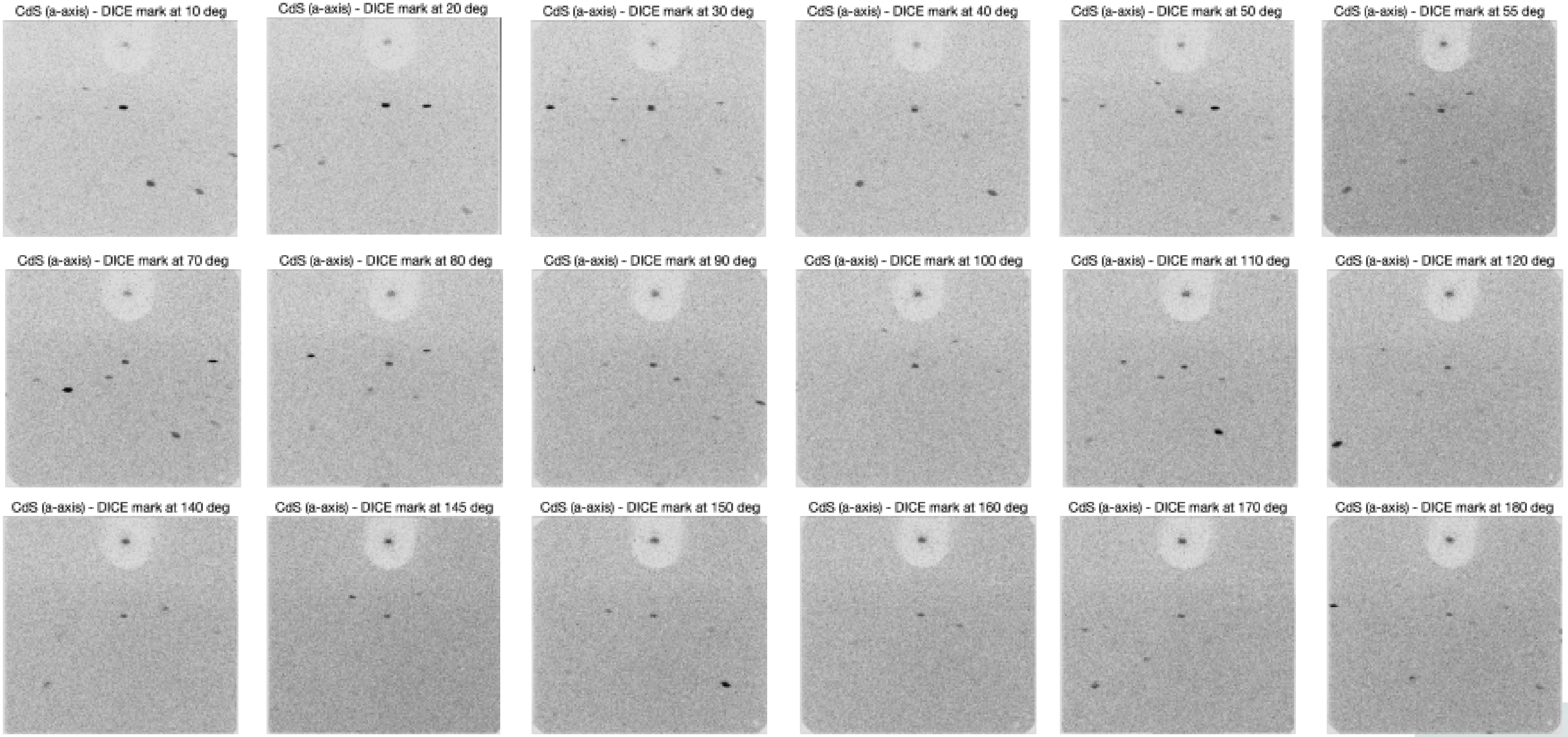
# Simulations comparable to Experiments



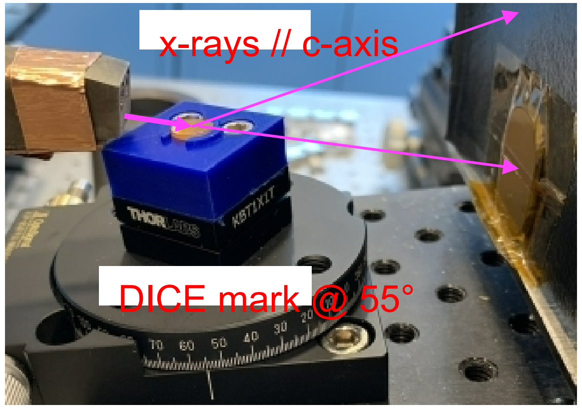

Thor diode data: Tom Ao, Dane Morgan

Ambient 180 rotation of CdS with a Molybdenum 17.6 keV k-$\alpha$ line source

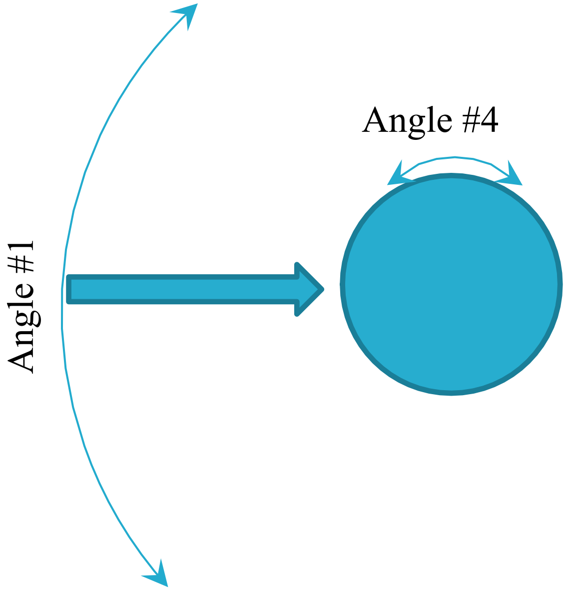


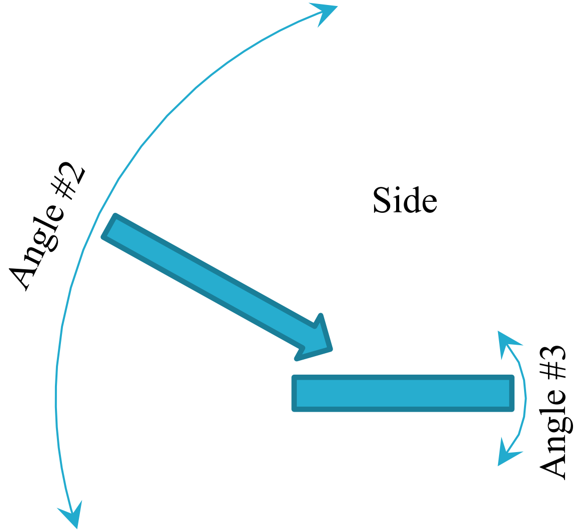
# Data created



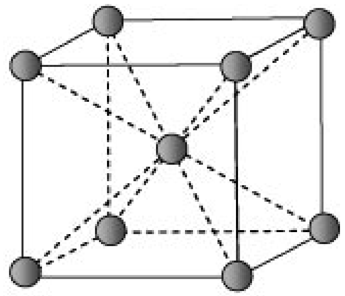

**Top view**



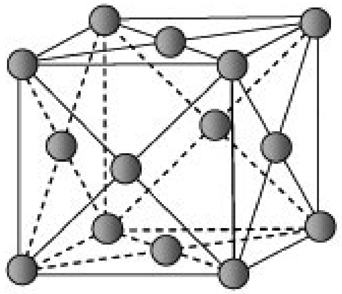

**Side view**



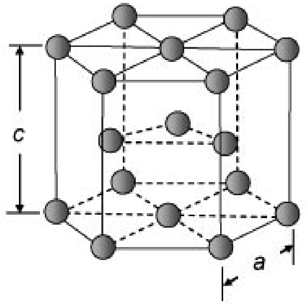
# Crystallography of solids & x-ray diffraction principles



Body centered cubic (bcc)

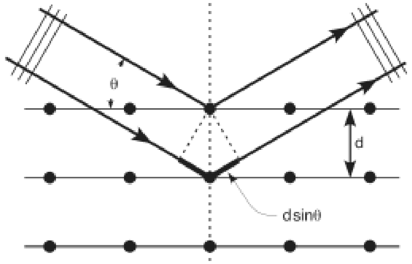


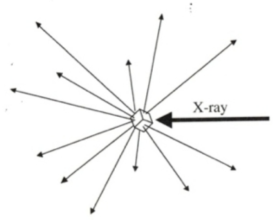
Face centered cubic (fcc)

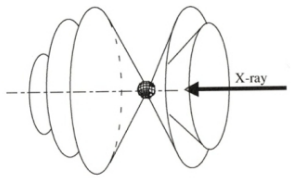



Hexagonal close-packed (hcp)

- Beam of x-rays strikes a crystal & scatters
- From angles and intensities of diffracted beams, 3-dimensional picture of the crystal is obtained




***Bragg's Law:***

Coherent reflections will occur for wavelength and crystal *d*-spacings that satisfy the condition:

$$n\lambda = 2d\sin\theta$$

The scattering angle (half-angle of the Debye-Scherrer cone) is:

$$\varphi = 2\theta$$

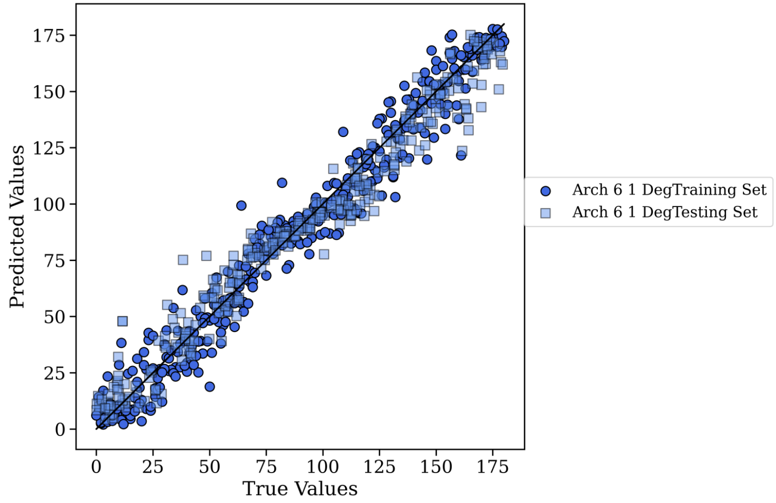
***Laue Spots:***

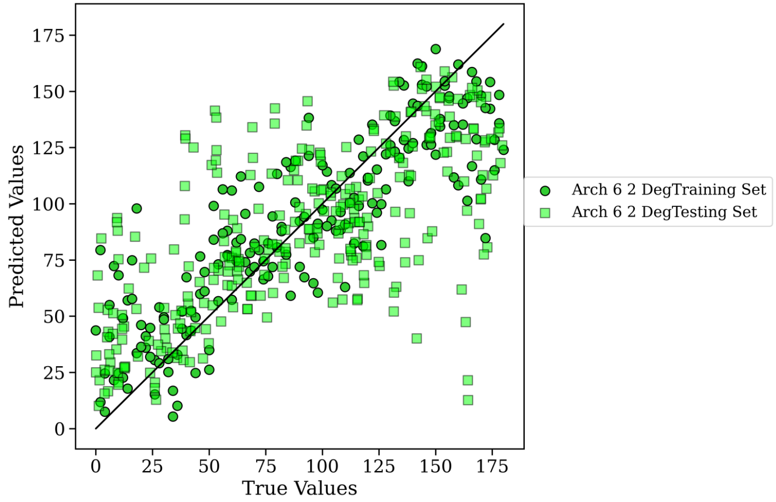
Illuminate a single crystal sample with a **continuum** x-ray beam, discrete reflections called **Laue spots** are observed.

***Debye-Scherrer Cones:***

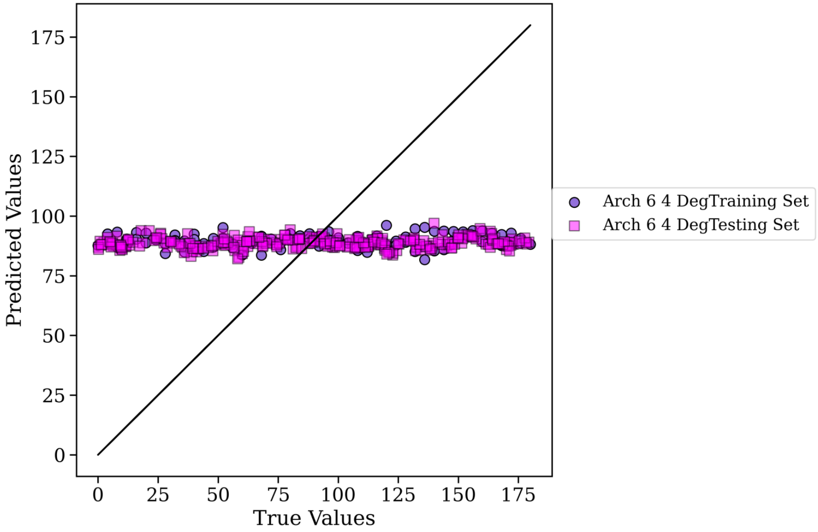
Illuminate a polycrystalline sample with a **monochromatic** x-ray beam, scattering patterns called **Debye-Scherrer cones** are observed.

## Network is able to learn

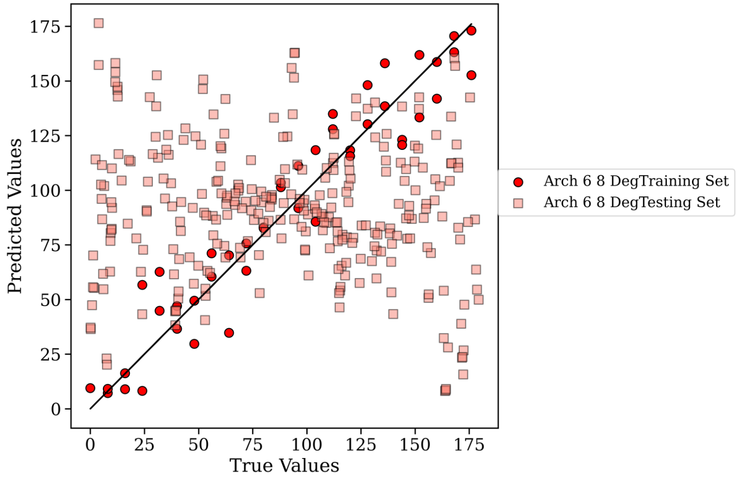


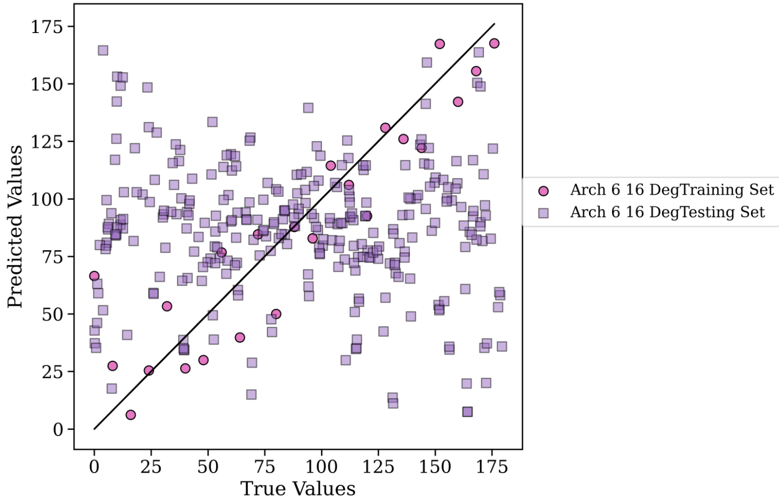



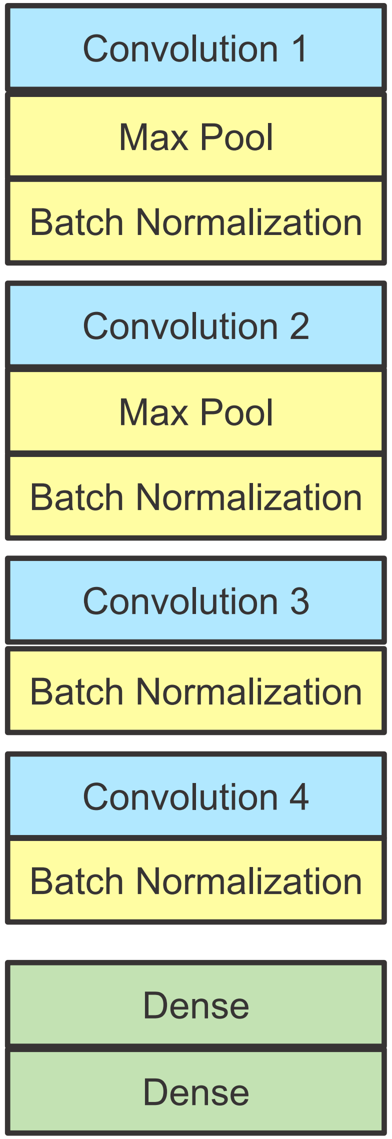

## Network is not able to learn




## Network becomes a ″look-up″ table




Convolution 1
Max Pool
Batch Normalization
Convolution 2
Max Pool
Batch Normalization
Convolution 3
Batch Normalization
Convolution 4
Batch Normalization
Dense
Dense