Physics Constrained Neural Net for Fast Approximate of Reflection High-Energy Electron Diffraction

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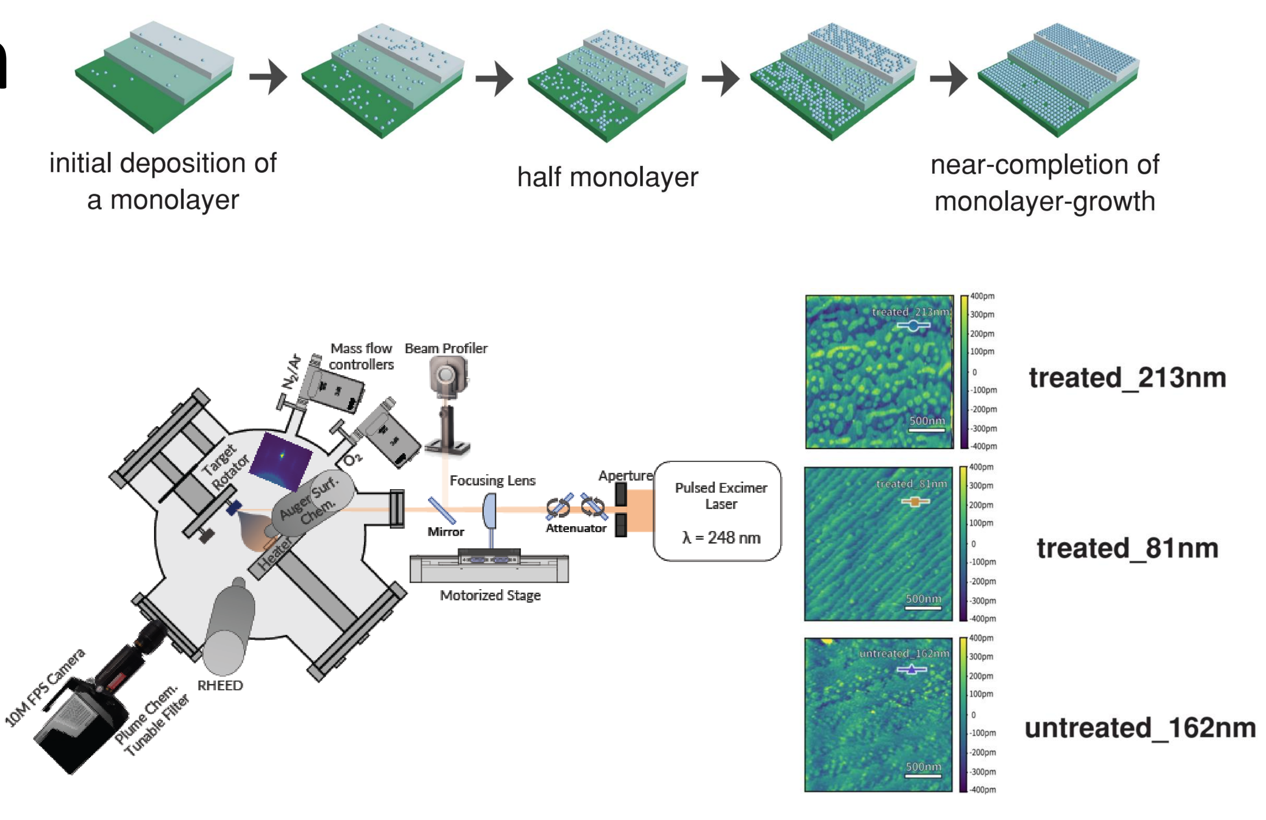
Pulsed Laser Deposition (PLD) is a widely used material science technique that deposits material onto a substrate. Reflection High Energy Electron Diffraction (RHEED) is commonly used to monitor the surface crystallinity of the deposited material. These techniques combined allow controlled growth for material fabrication. Typically, these systems rely on video cameras operating at 60-120hz, which fail to capture growth dynamics at practical deposition frequencies. By operating at 500hz, high-speed RHEED can provide real time insight into growth processes obscured by slower acquisition systems. Using this high-speed and information dense imagery has allowed the development of a neural net that can parameterize RHEED results in real time. This neural net is based on a physics-constrained LeNet5 that serves as a fast approximate for fitting RHEED. In the future, this model will be implemented on a Field Programmable Gate Array (FPGA) connected to the high-speed camera, allowing for real time control and adjustment of the testing devices.

Pulsed Laser Deposition

Pulsed laser deposition (PLD) is a technique where a high-power pulsed laser beam is focused inside a vacuum chamber to strike a target of the material that is to be deposited. This material is vaporized from the target (in a plasma plume) which deposits it as a thin film on a substrate.

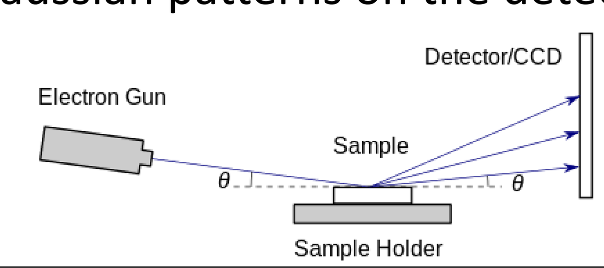
Using homoepitaxially deposited (001)-oriented $SrTiO_3$ as a model system, we demonstrate how high-speed RHEED can provide real time insight into growth processes obscured by slower acquisition systems.

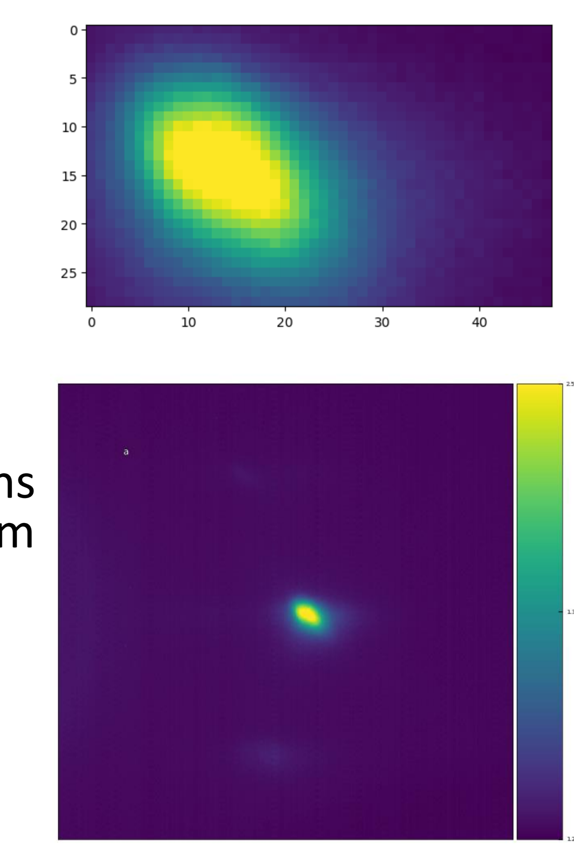


Reflection High Energy Electron Diffraction

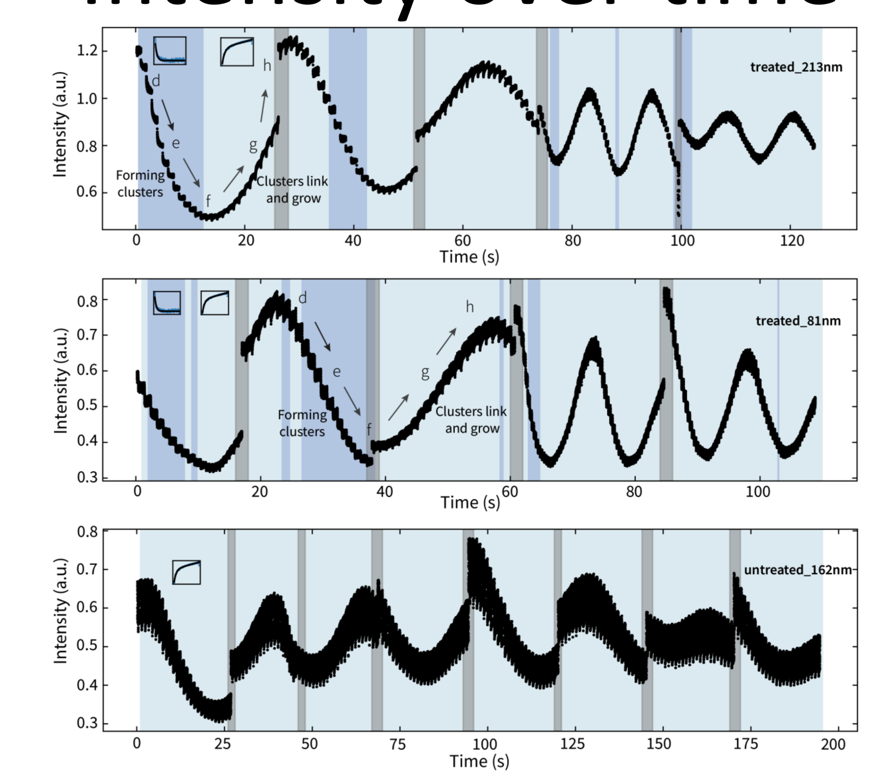
An electron gun generates a beam of electrons which strike the sample at a very small grazing angle to the sample surface

Incident electrons diffract from atoms at the surface of the sample, and the diffracted electrons interfere constructively at specific angles and form 2D Gaussian patterns on the detector.





Intensity over time

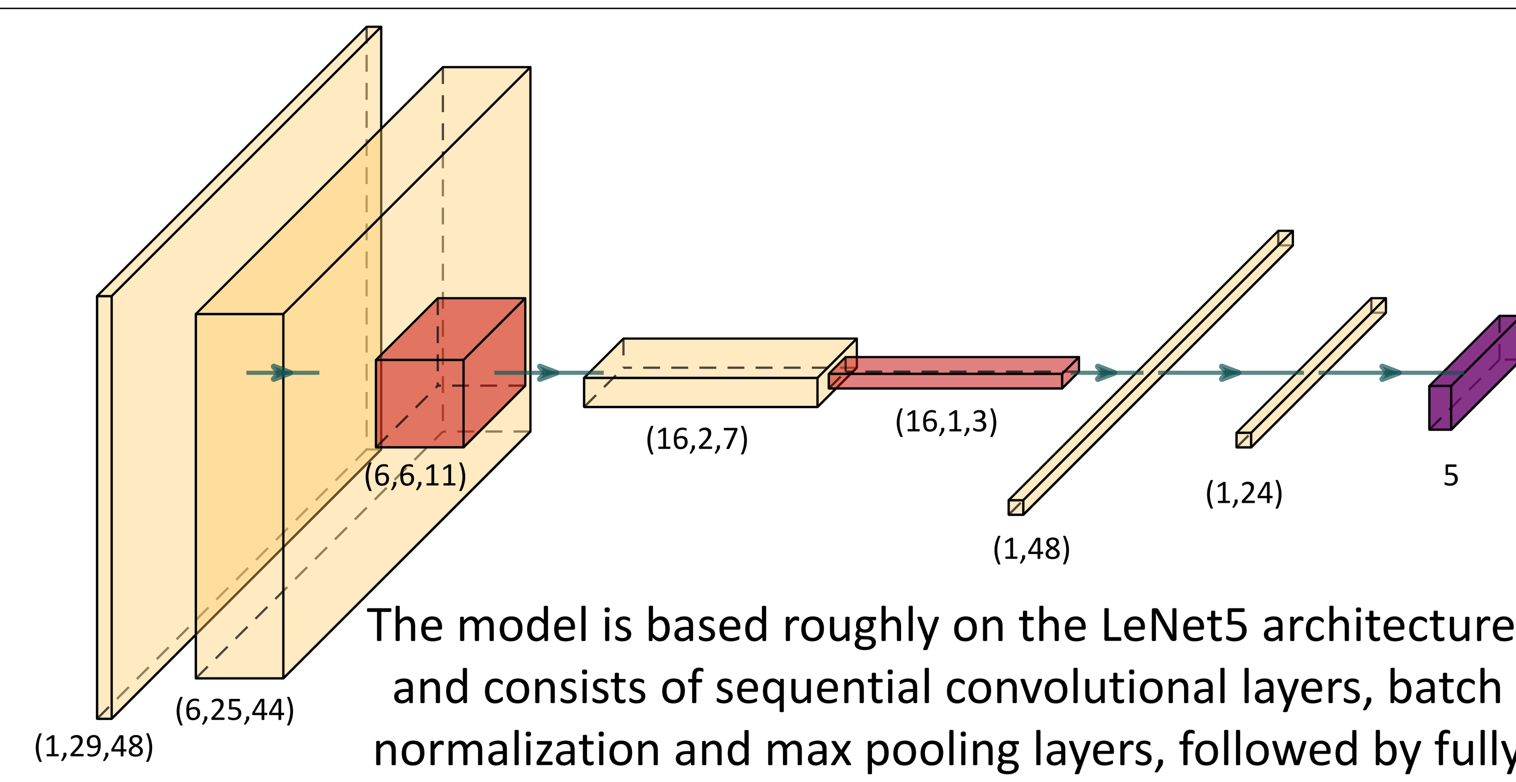


Model Setup

Preprocessing includes cropping to one spot and normalizing. The input size is (Batch Size, 1, 29, 48). Batch size is typically 1000 in training. There is one color channel. 29x48 is the cropped image size.

Embedding layer outputs 5 values that are 5 parameters to reconstruct a gaussian (Mean X, Mean Y, Covariance X, Covariance Y, Theta)

At inference time, the parameters are used to reconstruct a gaussian, serving as a decoder. This reconstruction is compared to the original with MSELoss.



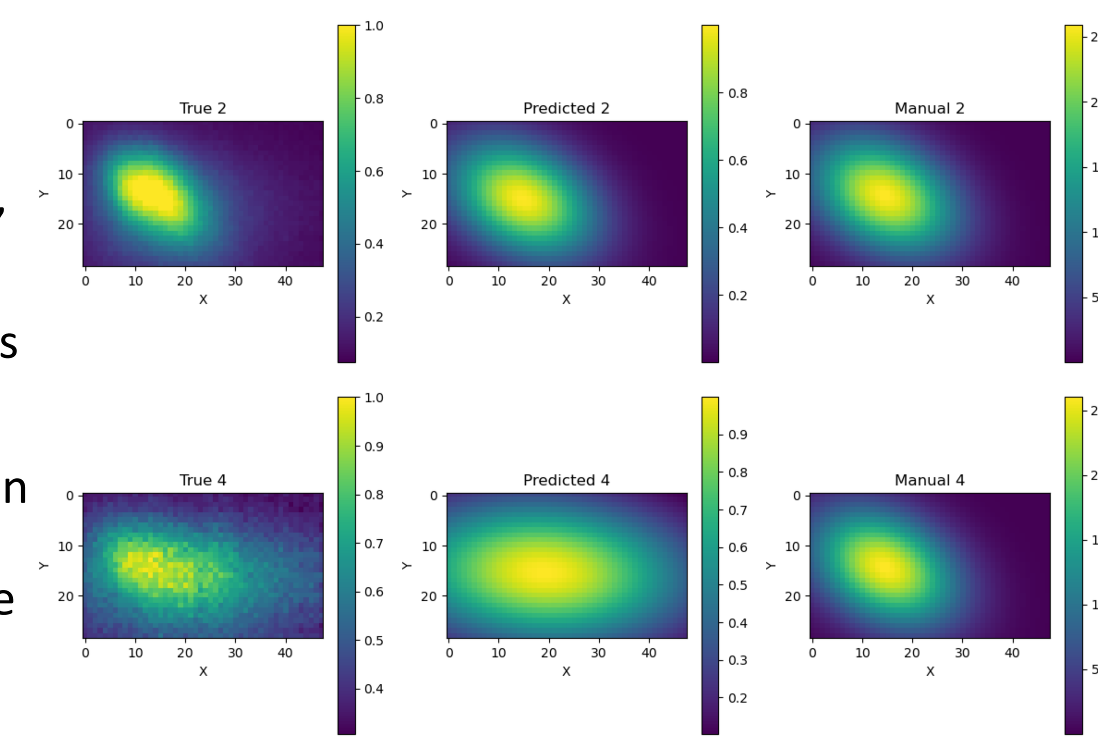
The model is based roughly on the LeNet5 architecture, and consists of sequential convolutional layers, batch normalization and max pooling layers, followed by fully connected layers reducing to 5 values.

Results

The predicted gaussian fits accurately to the true gaussian, loss of 0.009

Parameter count of 6269 allows for fast inference

Predicted fit adapts to changes in gaussian structure better than manual, which relies on average fitting.



Pytorch & HLS4ML

The model is built and trained in Pytorch.

HLS4ML is a Python package for machine learning inference in FPGAs

This tool allows for the conversion of my model written in Pytorch to a hardware language for FPGA deployment

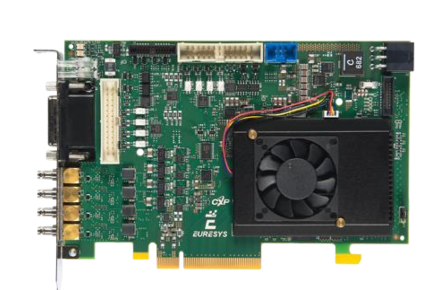
hls4ml PyTorch

Vivado & Frame Grabber

Vivado Design Suite is a software suite produced by Xilinx for synthesis and analysis of hardware description language designs

The device used is the Euresys Coaxlink Quad CXP-12, a frame grabber compatible with CustomLogic.

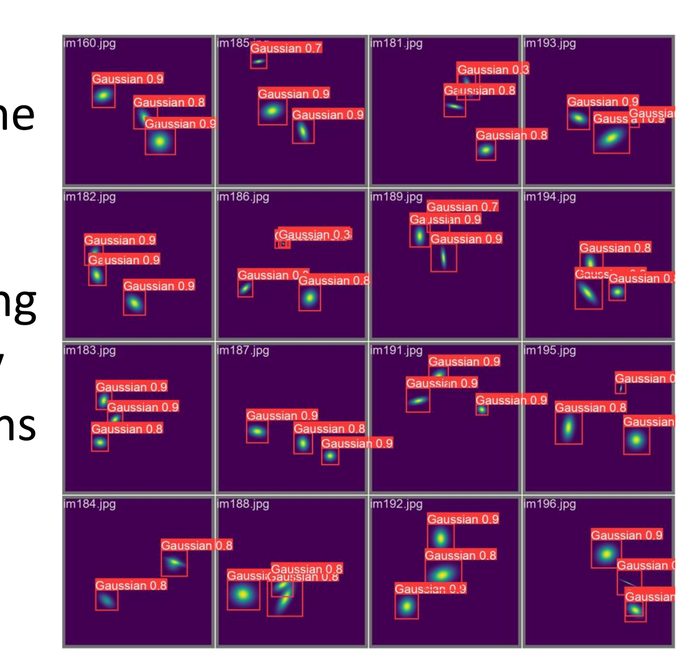
euresys Empowering Computer Vision



Future Work

Deployment onto a physical FPGA is the next major step for this project.

There is potential for an image cropping neural net using YOLOv5, to properly identify and crop the multiple gaussians on a RHEED pattern for individual analysis.



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Research was sponsored by the Army Research Laboratory and was accomplished under Cooperative Agreement Number W911NF-19-2-0119