In-Operando Tracking and Prediction of Transition in Material System using LSTM

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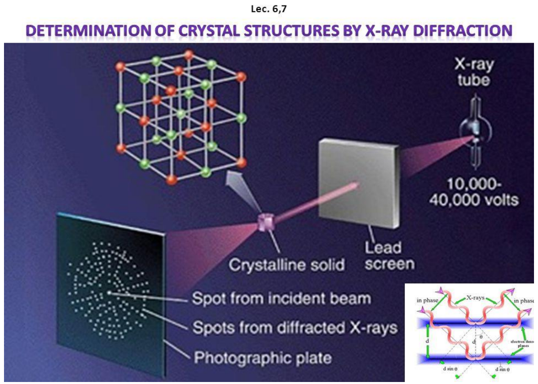
Background

A material system's structure is probed using x-ray scattering beams in NSLS-2.

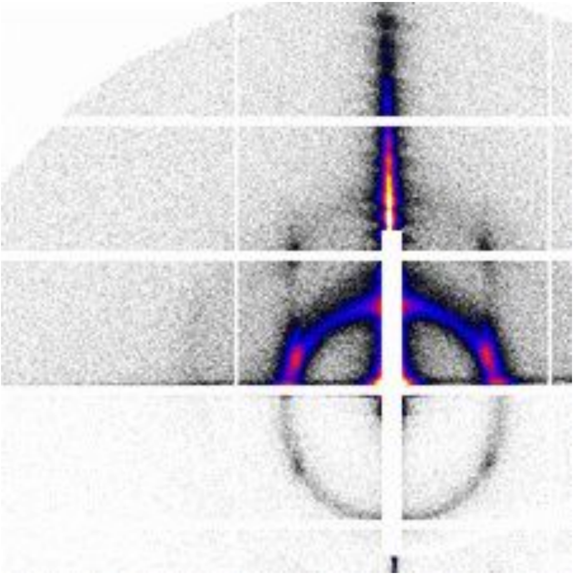


The structures of many material systems evolve as they are treated with physical processing.

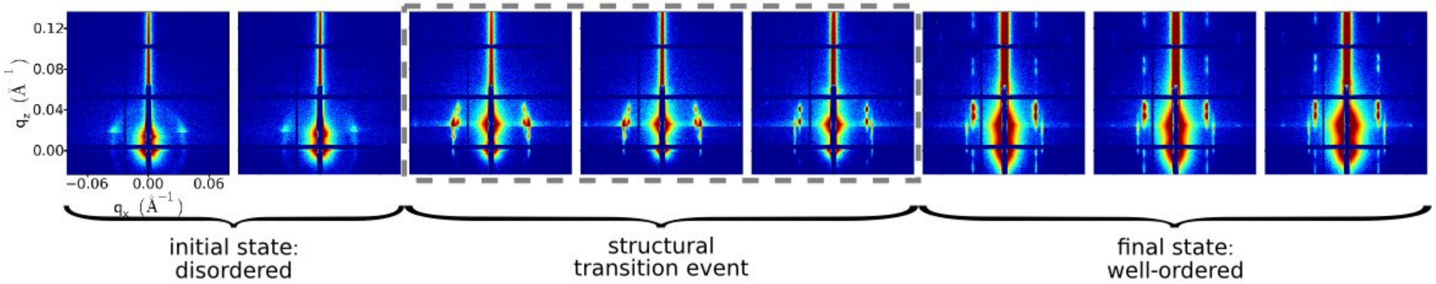
Background

Organic and Inorganic crystalline materials frequently coarsen over time as they are thermally treated with domains (grains) rotating and growing in size.

The **structural transition event** in a material system being probed under X-ray is the most information rich.



Background



In a material system undergoing the structural transformation, the peaks in the scattering images will sharpen and intensify, and the scattering rings will become increasingly ’textured’.

Motivation

Accurate identification of the transition frame in advance brings multiple benefits to the NSLS-II in-operando experiments such as:

- Minimal Beamline damage to samples
- Reduced Energy Costs
- Optimal sampling of material properties.

Approach

Formulate it as a **Future Frame Prediction** problem. (Sequence to Sequence)

Given a set of n images [X_1,X_2, .. X_n] from a video sequence, the objective is to predict (generate) the next m images [X^{n+1}, X^{n+2}, .. X^{n+m}] of the given video sequence as closely as possible to the ground truth frames [X^{n+1}, X^{n+2}, .. X^{n+m}].

Approach

We approach this problem in following two steps:

1. Identification of sequences having structural transition event.
2. Prediction of the future frame in the sequence based on historical image frames

We utilize an **LSTM** (Long Short-Term Memory) based model for this purpose.

Challenge

- Training an LSTM network (Deep Neural Network) requires a large amount of training data.
- Obtaining such amount of annotated training data from NSLS-2 is infeasible.

Solution

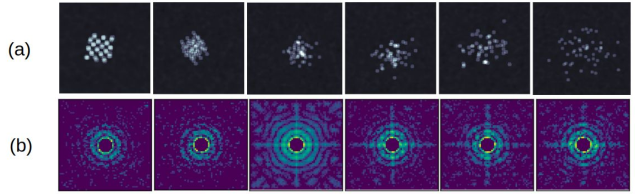
- Generate artificial data by simulating the diffraction process.

Synthetic Data

- Three crystal structures considered in our experiment namely BCC (Body-Centered Cubic), FCC (Face Centered Cubic) and SC (Simple Cubic) selected with random probability.

- A 3D box is filled with particles based on the chosen structure with particles location shifted by some random noise.

- Synthetic sequence of length 20-45 is obtained by repeatedly rotating the 3D box by a random angle.



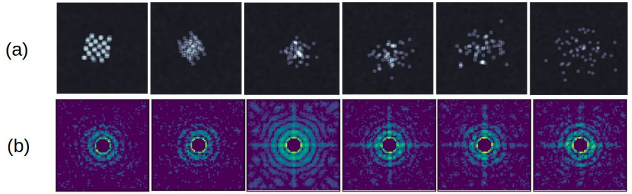
(a) Crystal structure
(b) X-ray scattering

Synthetic Data

- Index of Transition frame selected randomly. At the transition frame particles initiate to move in a random direction by some amount to simulate the Brownian motion.

- Structure is projected and FFT is applied on the 2D projection to obtain the magnitude image.

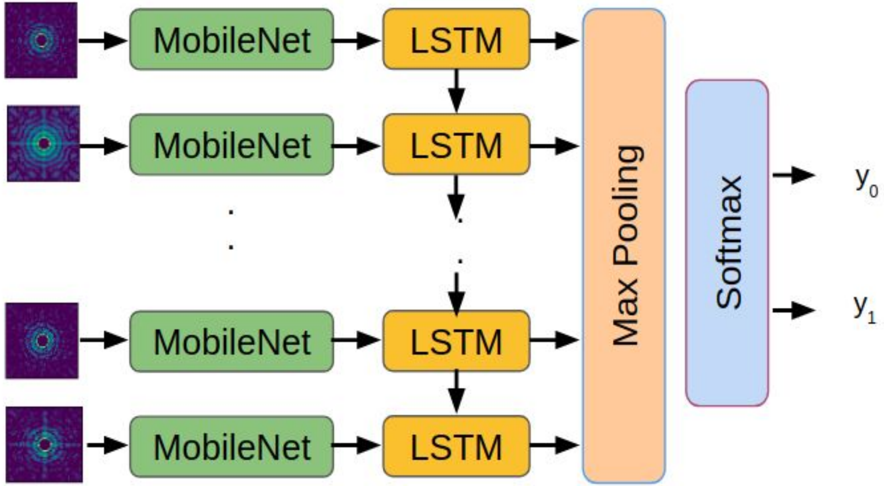
- 20k samples in the training split, with 10K samples containing transition frames and 10K samples without it. Similarly, 4800 samples were obtained in the testing split.



(a) Crystal structure
(b) X-ray scattering

Model

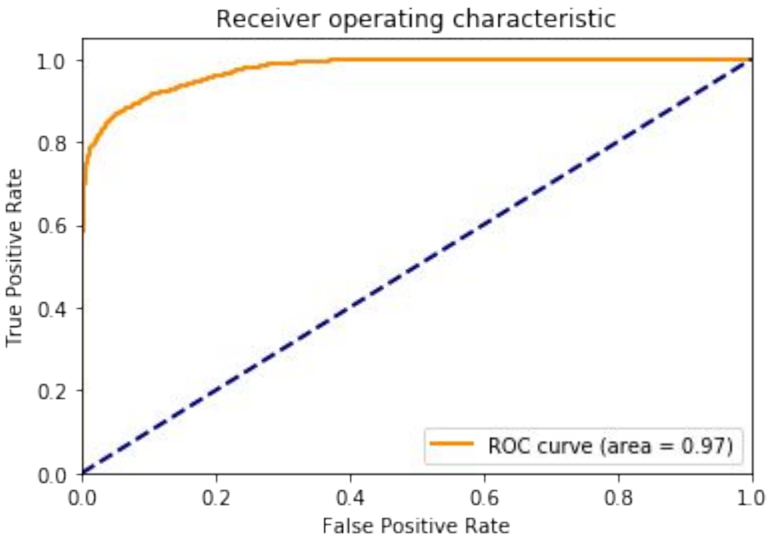
- We use a **CNN-LSTM**[1] model to exploit both temporal and spatial information.
- MobileNet CNN is used for doing transfer learning on the X-ray scattering images.



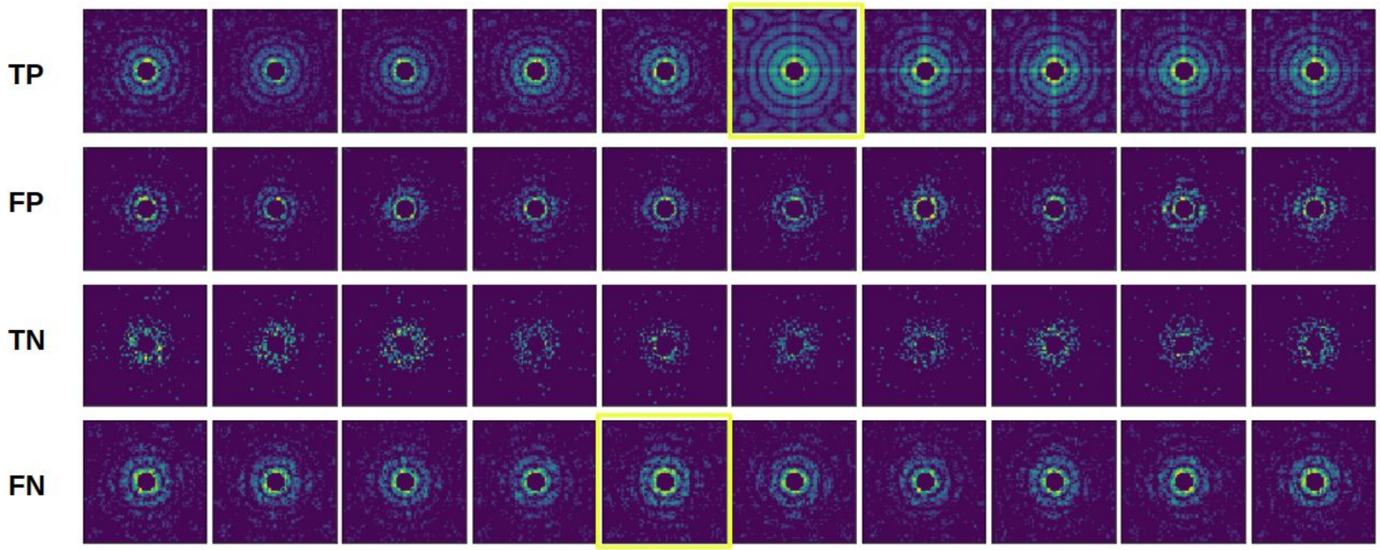
1. Beyond Short Snippets: Deep Networks for Video Classification

Results

- We obtain 0.97 AUC for a binary classification task (with transition sequence and without transition sequence)



Results



True Positive, False Positive, True Negative and False Negative from the test split

Future Work

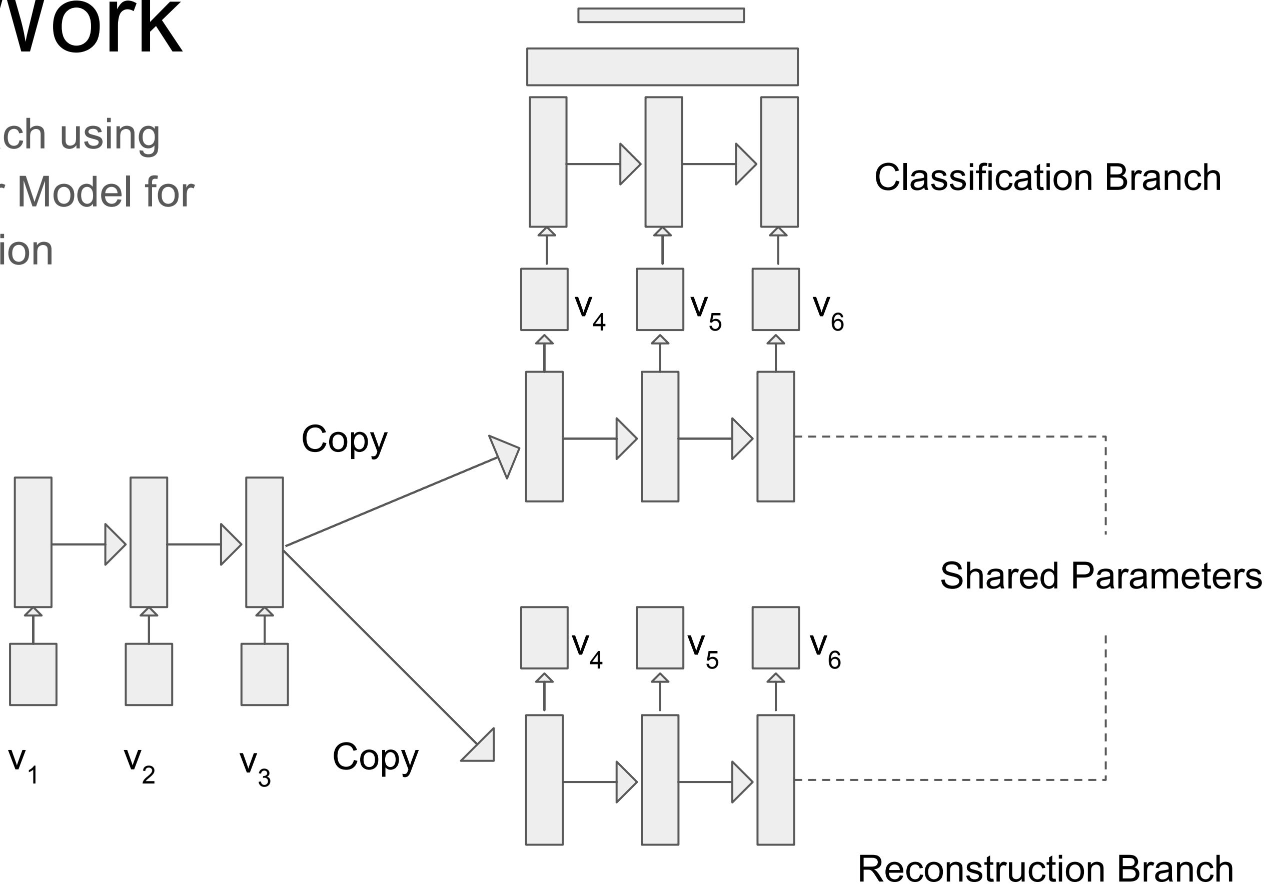
- Multi-task learning approach with the objectives to construct the future frames as well as identify the transition frame.

- Similar to an encoder-decoder model with two branches, one for classification and other for predicting (constructing) future frames[1].

1. Unsupervised Learning of Video Representations using LSTMs

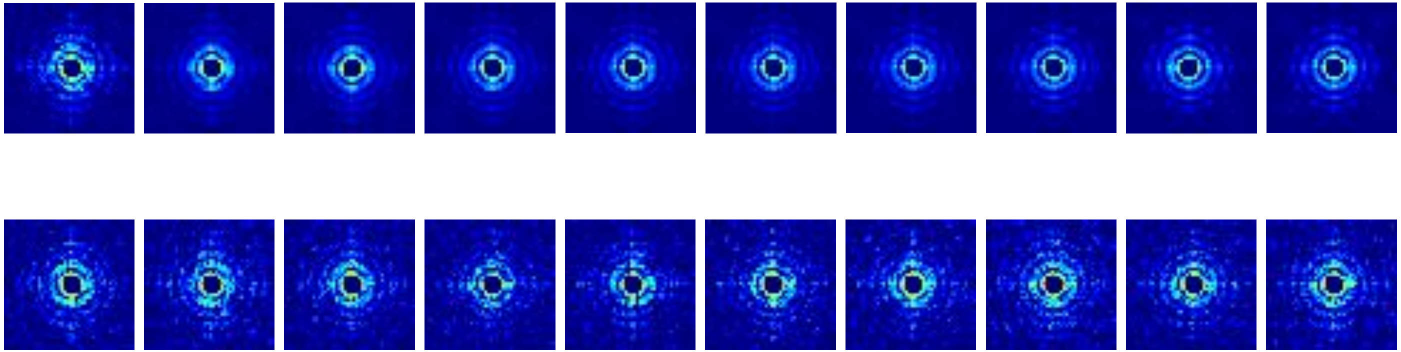
Future Work

Multi-task Approach using Encoder-Decoder Model for Transition prediction



Future Work

- Recently GAN based architectures have shown promising results in generating the future content[1] which could be incorporated in our model as well be replacing MSE loss by Adversarial loss.



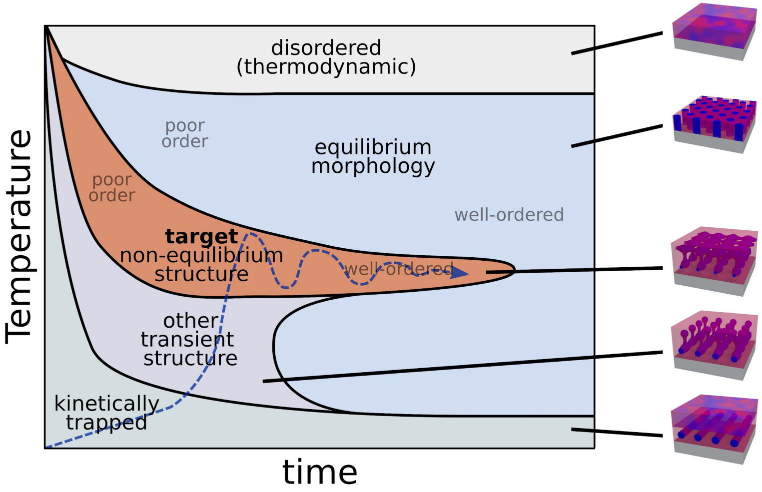
Constructed Sequence (MSE loss)

Real Sequence

1. Generating the future with adversarial transformers.

Future Work

Another direction to explore is to construct an autonomous agent to explore the state space. A computer-guided autonomous agent can select processing pathways during experimentation which can search for target states while avoiding transition to undesired states.



Thank You