AI QM Meeting Slides | Chen Group
2025/07/30

On ML Data Preparation *for* Quantum Material Growth

- **[Subtask 1]** (*Pre-Growth Annealing*) Image Classification on STO
- **[Subtask 2]** (*Post-Growth Annealing*) Reinforcement Learning for FeSe Film Growth

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Subtask 1: Pre-Growth Annealing to Prepare STO Substrate

- **Problem:** Identify if a given annealing condition yields a good reconstructed STO surface

- **Machine Learning (ML) Formulation:** Image Classification
  - **Input:** RHEED images (with annealing temperature and time?)
  - **Output:** surface quality label

- **Goals for today's discussion:**
  - Align our understanding of the Box data
  - Confirm specifications on additional data needed
  - Propose ML implementation details (*e.g.*, algorithms, neural network architectures)

Subtask 2: Post-Growth Annealing to Improve FeSe Film

- **Problem:** Learn a control policy that adjust annealing conditions for good FeSe films

- **ML Formulation:** Reinforcement learning, either offline or online
    - **Input:** A dataset of RHEED image sequence, annealing states, actions, and rewards
    - **Output:**
        - A learned (stepwise/trajectory-level) reward model
        - A learned policy to control annealing conditions

- **Goals for today's discussion:**
    - Align our understanding of the Box data and spreadsheets
    - Confirm specifications on data needed for (s, a, r, s') tuples for RL
    - Propose RL algorithms and implementation details

[Subtask 1 Discussion: STO Image Classification – Box/AI_QM/Data Understanding]

Dataset size: 2965 .bmp images under YYYY_MM_DD folders (containing films and/or substrates folders), and **2222** under .bmp images under RHEED_YangGroup folder.

- ➔ Which exact folder should be used for the image processing task?
- ➔ If we can increase the dataset size, how many more can we get?
- ➔ If we cannot increase the dataset size, is there any other similar datasets (in-house or open) we can use for pretraining?

Image Shape: the majority of images is **[3, 492, 656]**. (We can resize it to [3, 224, 224] for standard image processing with pretrained networks, or keep it and train from scratch.)

Label: N/A?

- ➔ Do we have all the labels for supervised training? If so, where is the path or how do they correspond to images?
- ➔ If we do not have labels:
  - ◆ (partial labeling) How many can we have them labeled by humans? How long would it take?
  - ◆ (contrastive learning) Otherwise, if we only have good/bad examples, what would be the ratio?

[Subtask 1: STO Image Classification – Implementation Details]

Network Architecture: Depending on the total dataset size, we can use the following architectures:

- CNN module (AlexNet/**ResNet-18**/ResNet-32)
- Attention module (**ViT**/ConvNeXT/SwinT, if we can get more RHEED data or similar data for pretraining)
- Vision Language Models (LLaVA/MiniGPT-4/PaliGemma)
    - The task will become captioning instead of classification, and we may integrate actions, like piO.

Algorithm: Depending on the label type, we can consider following algorithms:

- Supervised: using standard cross-entropy loss.
- Semi-Supervised:
    - Case 1: partial labeling (in general, we can do pseudo-labeling)
    - Case 2: contrastive learning with some labeled examples, using distance as discriminative signals

Current Progress:

- Finished standard processing with torch models of ResNet-18; using standard image pretraining (e.g., rotation prediction, JEPA) however there is no downstream tasks with labels. If the labels are available, the training can be completed within hours.

[Subtask 2: Annealing Control – RL Data Specification]

In general, we need $(o_{t}, a_{t}, o_{t+1}, r_{t})$ tuple at every time step t. That is, we see observation o_t (), take action a_t, then transit to a new state and get a new observation o_{t+1}, with or without a numeric reward r_t.

State / Observation:

- RHEED image

➔ What else? Do we need to condition on different stage/mode or any other external signals?
➔ Is the initial state an RHEED image, or something related to subtask 1?
➔ How long is an episode (i.e., one round of experiment)?

Action:

- annealing temperature, annealing duration

➔ What else? What are their parameter space?

Reward:

- Before termination: a function of the RHEED image (like labels)?
- At termination: combined function of the final RHEED image and other measurements that evaluate the quality.

Network Architecture:

- We can keep the same CNN or ViT encoder from subtask 1 as the visual backbone for this subtask.

Algorithm:

- **Offline RL:** Behavioral Cloning, Conservative Q-Learning, Decision Transformer, etc.
- **Online RL:** REINFORCE, SAC, or model-based RL, etc.

[Appendix: Jargon List for Both's Reference]

FeSe	A material made of iron (Fe) and selenium (Se). It can become superconducting under certain conditions.
Thin Film	A very thin layer of material, often only a few atoms thick, grown on top of another material.
Substrate	The solid surface on which a thin film is grown.
STO ($SrTiO_3$)	A commonly used substrate material for growing thin films.
Epitaxy	A process for growing a crystal layer where atoms line up with the atoms of the underlying substrate.
Annealing	Heating a material to a certain temperature and holding it there for some time to improve its structure.
Flux	The rate at which atoms are supplied during growth. It controls how much of each element gets deposited.
RHEED	Reflection high-energy electron diffraction. A method that shoots electrons at a material's surface to get a diffraction pattern. The pattern helps analyze how well the material is growing.
Offline RL	The case when the reinforcement learning agent learns a policy from a fixed, pre-collected, reward-labeled dataset w/o further interaction with the environment.
Online RL	The agent learns by interacting with the environment in real time, collecting new data and get real-time reward.