Automatically Aligning Crystals to Neutron Diffraction Instruments Using Reinforcement Learning

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The Problem Statement

This project helps address the ongoing problem of the large amounts of time aligning can take, as experimenters often take guesses on the structure of the crystal. In addition to this neutron diffraction experiments requiring extensive amounts of firing time. Finally, there are only two U.S. locations that house neutron generators that can facilitate neutron diffraction leading to limited reservations. Speeding up the neutron diffraction process by automating it would help lead to faster experiments

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Methods

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Reinforcement Learning

•Agent - The algorithm/function in the model that performs the task
•Environment - The world in which the agent carries out its actions
•State - The situation of the agent in an environment
•Action - The moves that are chosen
•Reward - Feedback for the agent's actions in a given state

Advantages –

•Can be used to solve very complex problems
•Can outperform humans in many tasks
•It is similar to the learning of human beings and can correct errors during the training process
•It doesn't require large labeled datasets

Q Learning

•Model-free reinforcement learning algorithm
•Contains a Q-table that stores the expected rewards for state-action pairs (Q-values)
•Q-values updated iteratively over multiple training episodes
•Agent selects the action with the highest Q-value
•Effective for small state spaces
•Different from Value function in that value functions are rewarded based on the current state of the agent, while q functions are rewarded based on the agents chosen action in a certain state

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Steps

1.Build the q learning algorithm
2.Train the algorithm using simulated data
3.Evaluate/test the algorithm
4.Tune hyperparameters if needed
5.Evaluate again

•Training:
- Reward
  - Punished for each rotation
  - Awarded for finding peak

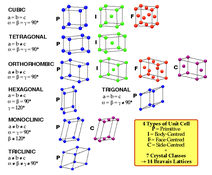
•Model decides how much to rotate
•Rotates automatically until finds diffraction peak

Background

Crystallography

Crystals

•A type of solid material composed of atoms or groups of atoms that are arranged in a three-dimensional pattern that is very ordered
•Lattice determines the different diffraction patterns



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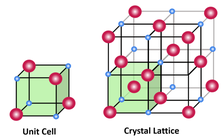
Crystal Lattice and Unit Cell



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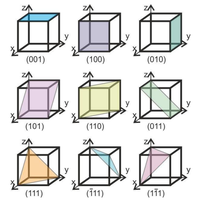
Bravais Lattice

•Symmetrical three-dimensional structural arrangements
•One of the 14 different types of unit cells that a crystal structure can be made up of
•Determines the different diffraction patterns



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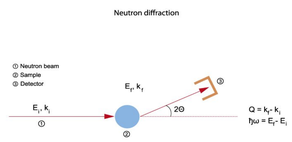
Crystallographic Planes (Miller Indices, HKL)

- Represent the orientation of crystallographic planes within the crystal lattice
- The certain plane for alignment is chosen by the experimenter

Neutron Diffraction

•Neutron Diffraction is the application of neutron scattering to determine the atomic and magnetic structure of a material
•A sample is placed in a beam of neutrons to obtain a diffraction pattern that provides information about the structure of the sample



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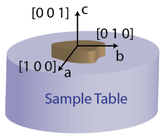
Alignment

Alignment

1.Choose a particular plane
2.Choose two projection vectors corresponding to the plane
3.Rotate table
4.Take alignment scans
5.Analyze scans
6.Repeat 3, 4, and 5 until aligned



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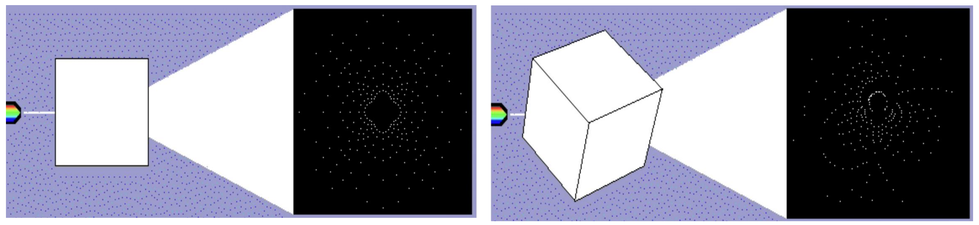
Two different alignments providing different scattering patterns



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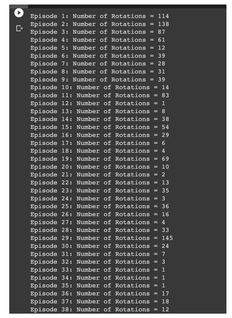
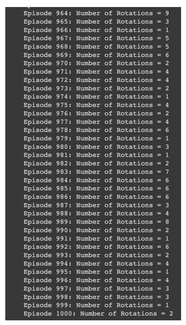
Results

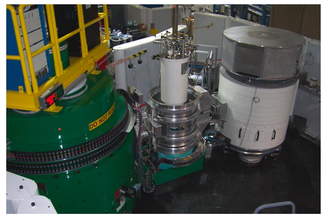
My Q-learning algorithm worked well in this situation. The number of rotations needed to find a peak decreased overall after hundreds of episodes.





Future Work

Implement mcstas to simulate what we expect to observe on an instrument at certain crystal orientations to make the model more realistic. The program also needs to be implemented to certain instruments such as a triple-axis spectrometer



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