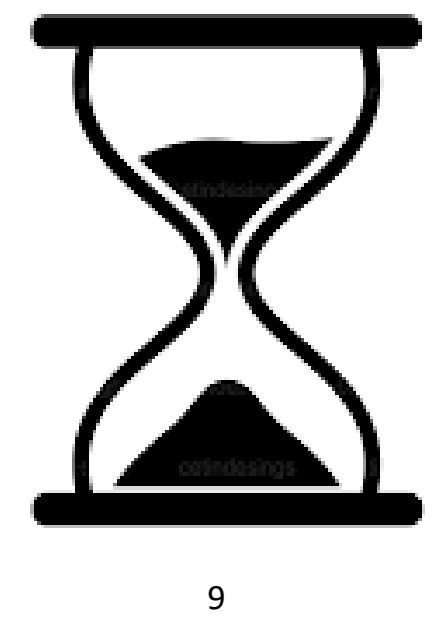


## The Problem Statement

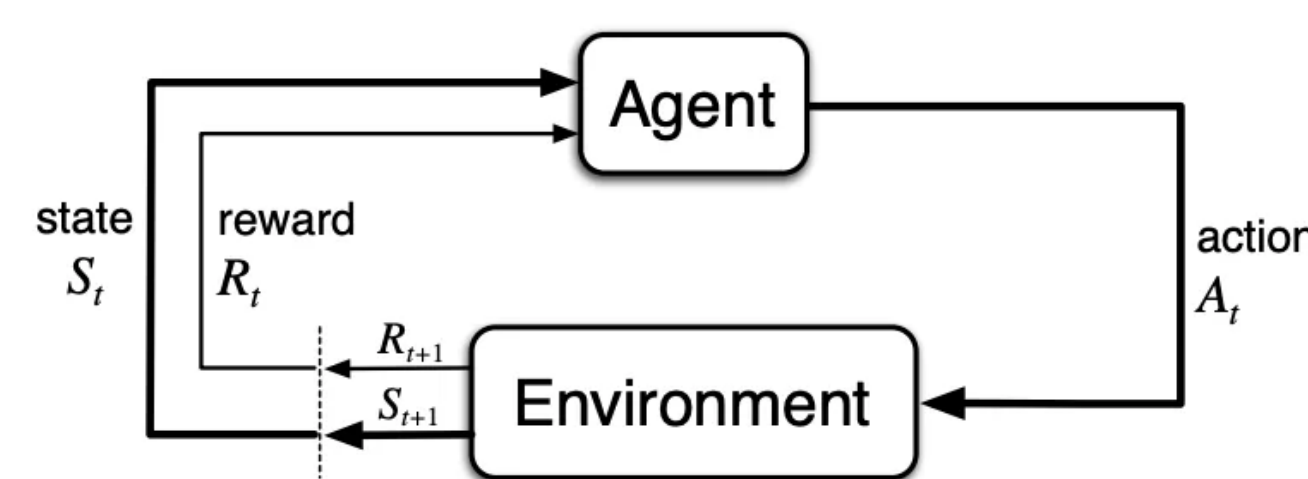
This project helps address the ongoing problem of the large amounts of time aligning can take, as experimenters often take guesses on the structure of the crystal. In addition to this neutron diffraction experiments requiring extensive amounts of firing time. Finally, there are only two U.S. locations 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



## Methods

### 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

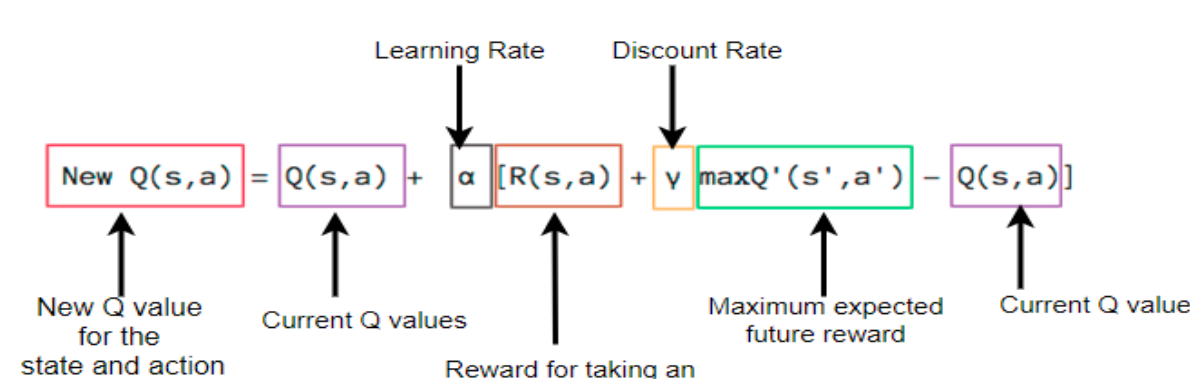


### Advantages -

- 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



### Steps

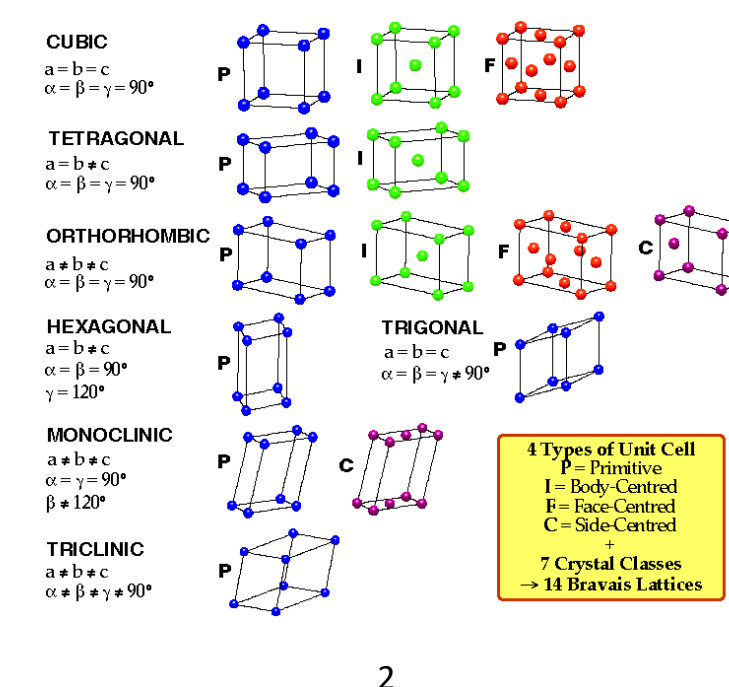
1. Build the q learning algorithm
  2. Train the algorithm using simulated data
  3. Evaluate/test the algorithm
  4. Tune hyperparameters if needed
  5. Evaluate again
- Training:
    - Reward
    - Punished for each rotation
    - Awarded for finding peak
  - Model decides how much to rotate
  - Rotates automatically until finds diffraction peak

## Background

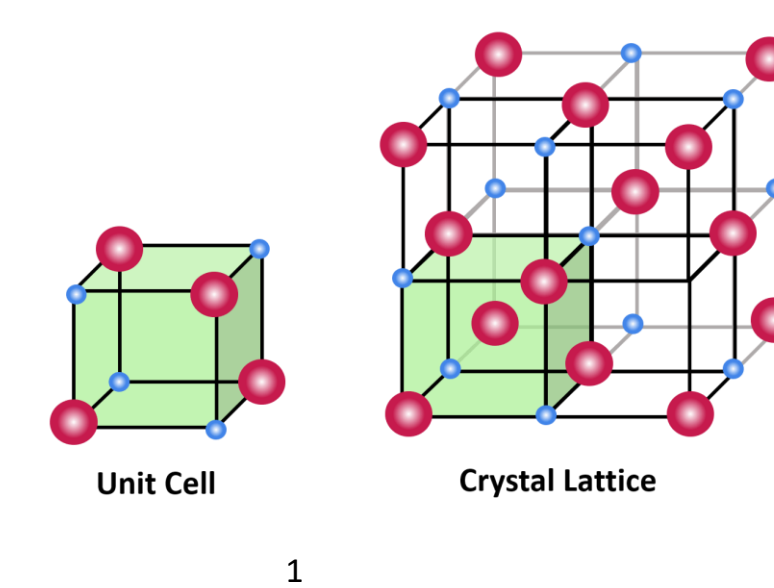
### Crystallography

#### 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

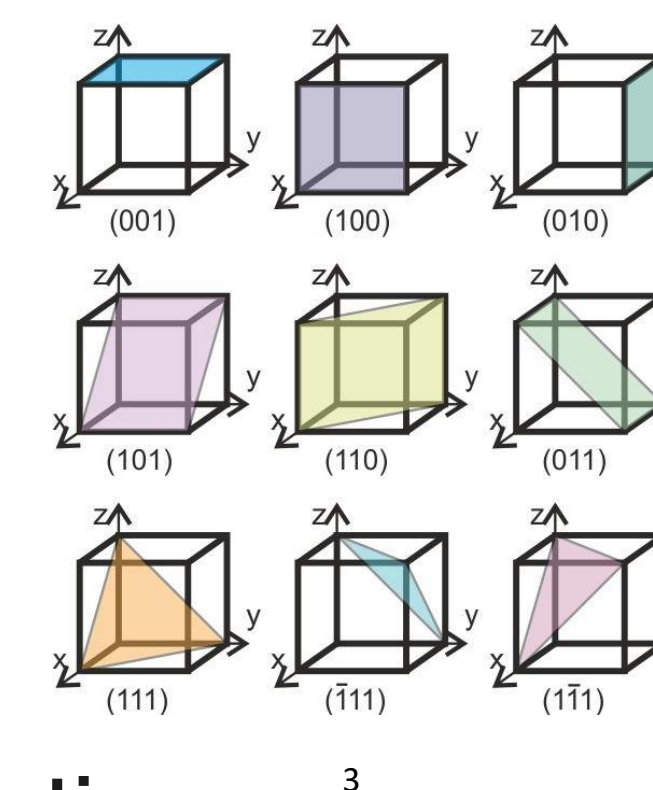


#### Crystal Lattice and Unit Cell



#### Bravais Lattice

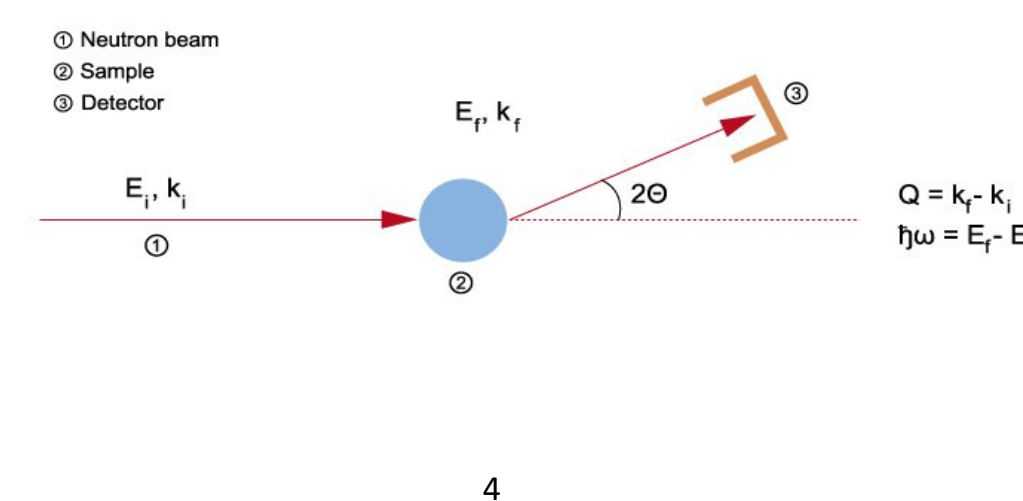
- Symmetrical three-dimensional structural arrangements
- One of the 14 different types of unit cells that a crystal structure can be made up of
- Determines the different diffraction patterns



#### 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



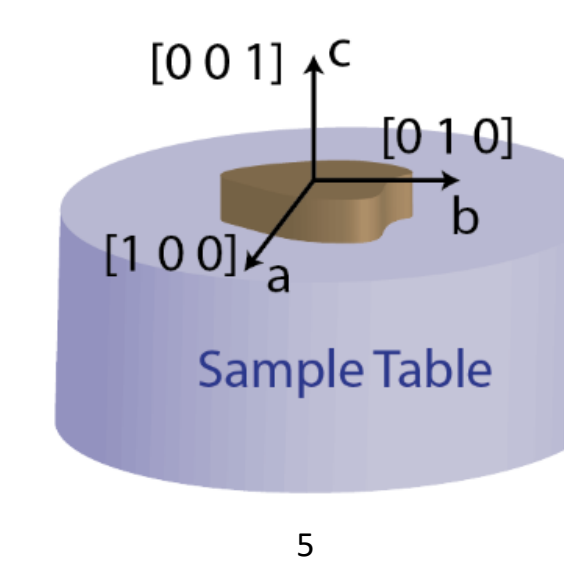
#### Neutron Diffraction

- 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

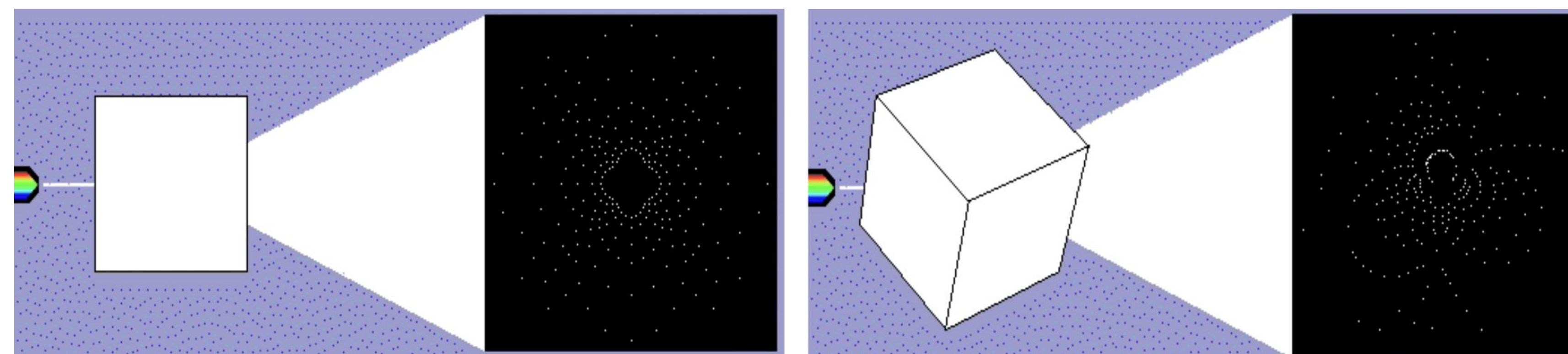
### Alignment

#### 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



#### Two different alignments providing different scattering patterns



## 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.

Episode 11: Number of Rotations = 114
Episode 12: Number of Rotations = 118
Episode 13: Number of Rotations = 87
Episode 14: Number of Rotations = 65
Episode 15: Number of Rotations = 12
Episode 16: Number of Rotations = 28
Episode 17: Number of Rotations = 31
Episode 18: Number of Rotations = 39
Episode 19: Number of Rotations = 14
Episode 20: Number of Rotations = 83
Episode 21: Number of Rotations = 1
Episode 22: Number of Rotations = 8
Episode 23: Number of Rotations = 38
Episode 24: Number of Rotations = 14
Episode 25: Number of Rotations = 29
Episode 26: Number of Rotations = 49
Episode 27: Number of Rotations = 4
Episode 28: Number of Rotations = 10
Episode 29: Number of Rotations = 2
Episode 30: Number of Rotations = 13
Episode 31: Number of Rotations = 35
Episode 32: Number of Rotations = 3
Episode 33: Number of Rotations = 16
Episode 34: Number of Rotations = 14
Episode 35: Number of Rotations = 4
Episode 36: Number of Rotations = 145
Episode 37: Number of Rotations = 24
Episode 38: Number of Rotations = 7
Episode 39: Number of Rotations = 1
Episode 40: Number of Rotations = 5
Episode 41: Number of Rotations = 1
Episode 42: Number of Rotations = 17
Episode 43: Number of Rotations = 18
Episode 44: Number of Rotations = 13

Episode 44: Number of Rotations = 9
Episode 45: Number of Rotations = 3
Episode 46: Number of Rotations = 1
Episode 47: Number of Rotations = 5
Episode 48: Number of Rotations = 5
Episode 49: Number of Rotations = 6
Episode 50: Number of Rotations = 2
Episode 51: Number of Rotations = 4
Episode 52: Number of Rotations = 4
Episode 53: Number of Rotations = 2
Episode 54: Number of Rotations = 1
Episode 55: Number of Rotations = 4
Episode 56: Number of Rotations = 6
Episode 57: Number of Rotations = 1
Episode 58: Number of Rotations = 3
Episode 59: Number of Rotations = 4
Episode 60: Number of Rotations = 2
Episode 61: Number of Rotations = 7
Episode 62: Number of Rotations = 6
Episode 63: Number of Rotations = 6
Episode 64: Number of Rotations = 6
Episode 65: Number of Rotations = 6
Episode 66: Number of Rotations = 6
Episode 67: Number of Rotations = 3
Episode 68: Number of Rotations = 4
Episode 69: Number of Rotations = 8
Episode 70: Number of Rotations = 2
Episode 71: Number of Rotations = 1
Episode 72: Number of Rotations = 1
Episode 73: Number of Rotations = 6
Episode 74: Number of Rotations = 2
Episode 75: Number of Rotations = 2
Episode 76: Number of Rotations = 4
Episode 77: Number of Rotations = 4
Episode 78: Number of Rotations = 6
Episode 79: Number of Rotations = 6
Episode 80: Number of Rotations = 3
Episode 81: Number of Rotations = 4
Episode 82: Number of Rotations = 8
Episode 83: Number of Rotations = 2
Episode 84: Number of Rotations = 1
Episode 85: Number of Rotations = 6
Episode 86: Number of Rotations = 2
Episode 87: Number of Rotations = 4
Episode 88: Number of Rotations = 4
Episode 89: Number of Rotations = 4
Episode 90: Number of Rotations = 3
Episode 91: Number of Rotations = 1
Episode 92: Number of Rotations = 2
Episode 93: Number of Rotations = 1
Episode 94: Number of Rotations = 6
Episode 95: Number of Rotations = 2
Episode 96: Number of Rotations = 4
Episode 97: Number of Rotations = 4
Episode 98: Number of Rotations = 1
Episode 99: Number of Rotations = 1
Episode 100: Number of Rotations = 2

## 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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