Automating the Alignment of Crystals

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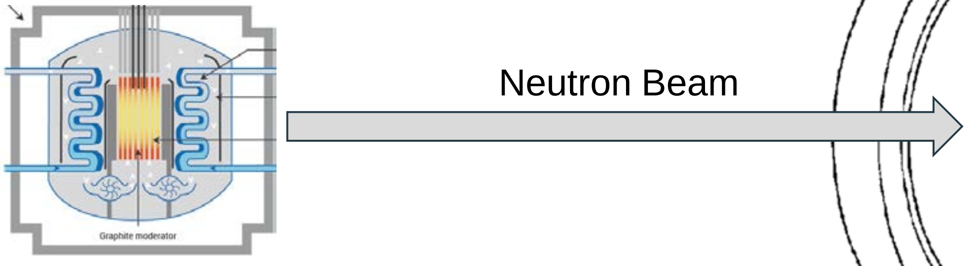
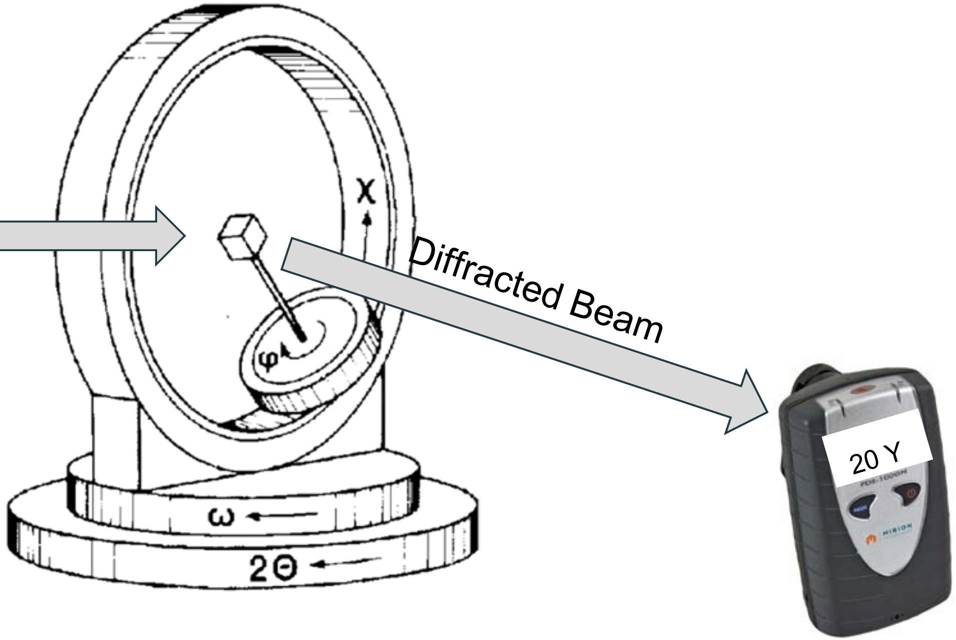
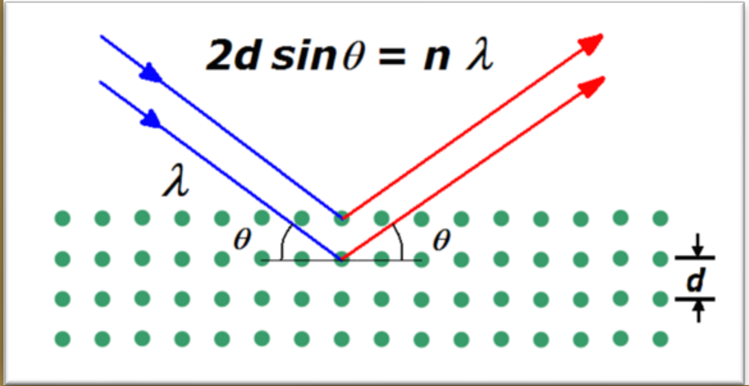
Background

- The structure of crystals help scientist understand its properties
- Crystal must be aligned to determine its orientation
- These features can be hard to find for various reasons
- Strontium Titanate ($SrTiO_3$), for example
  - Simple cubic geometry
  - Obtains a large dielectric constant at cold temperatures
  - Becomes a superconductor at 0.35 K


Graphite moderator
Neutron Beam

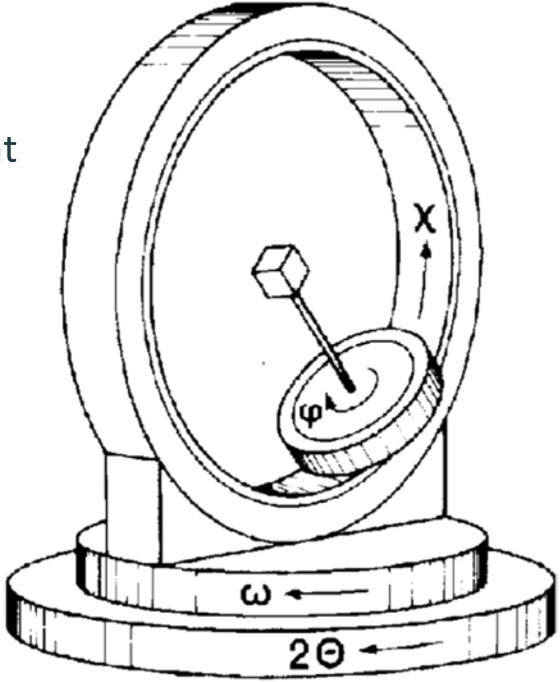

Diffracted Beam
χ
φ
ω
2Θ
20 Y


$2d \sin\theta = n\lambda$
λ
θ
θ
d

Common Vocabulary

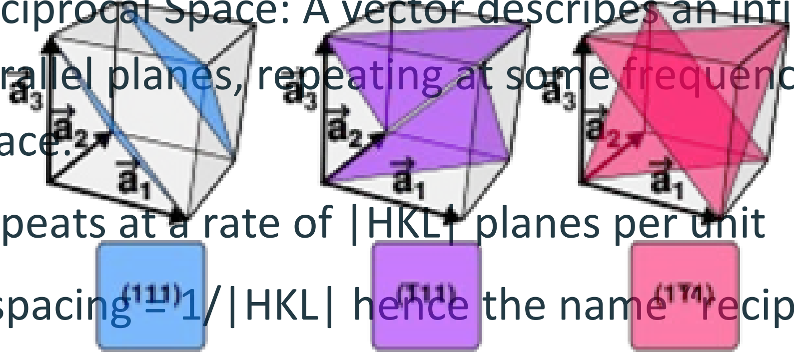
- Reflection: an instance of neutrons hitting the detector
- Diffracting Position: a specific orientation of the crystal that results in a reflection
- Rotation Axis: Phi (ϕ), Chi (X) , Omega (Ѡ) → rotation matrix (R)
- Detector Angles: TwoTheta (2Θ)

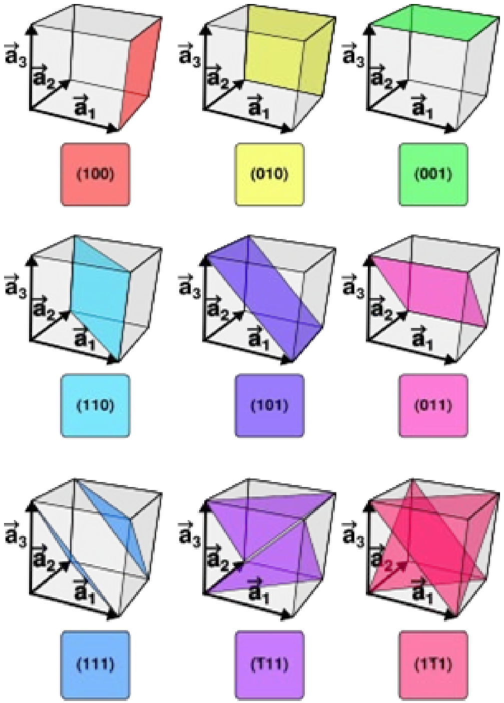
- HKL vectors and the UB matrix
    - More on these later



HKLs and Miller Indices

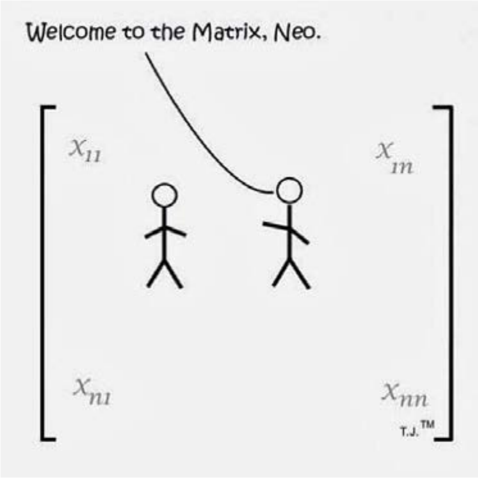
- Reciprocal Space: A vector describes an infinite set of parallel planes, repeating at some frequency in real space.
- Repeats at a rate of |HKL| planes per unit
- d spacing = 1/|HKL| hence the name "reciprocal"
- Allows us to define which set of faces we are looking at



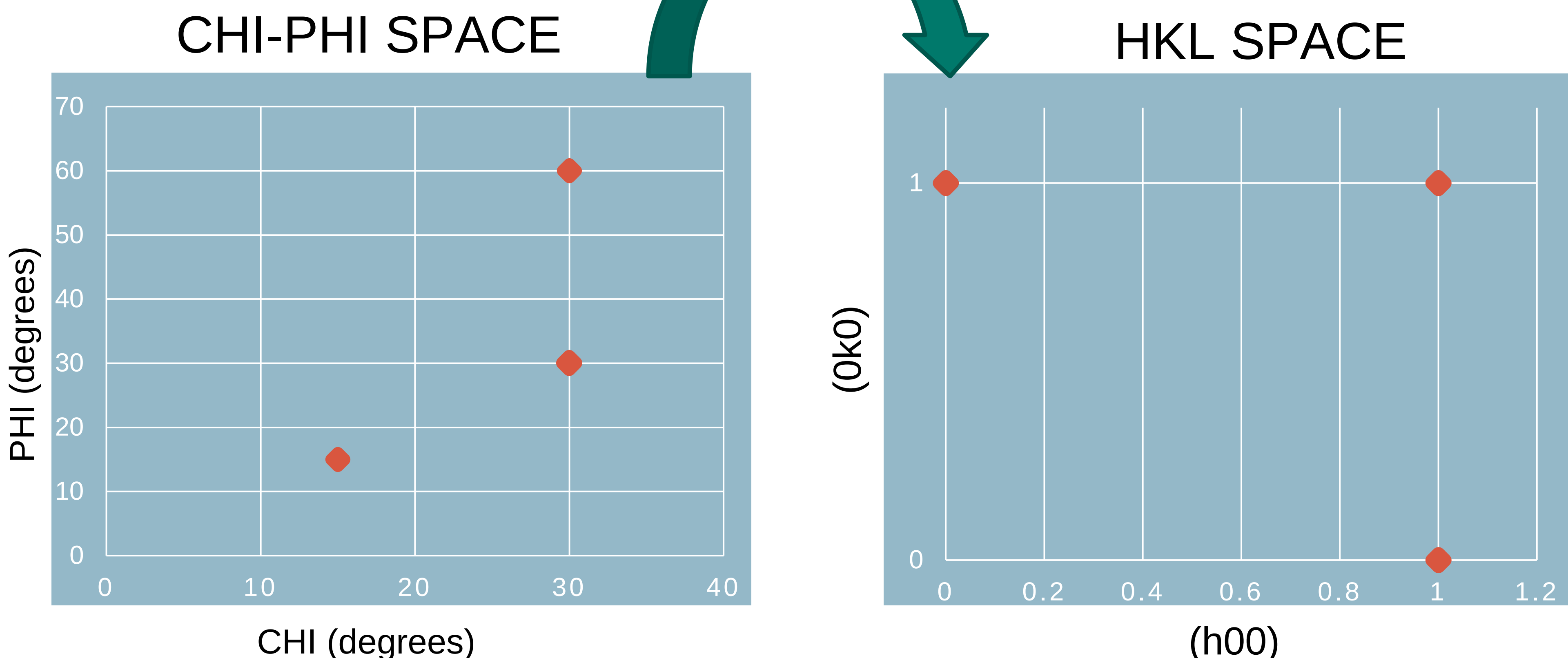


UB Matrix

- The UB Matrix allows scientist to figure out what motor angles (X, ϕ, Ѡ, 2Θ) are needed to hit any desired reflection
- In order to calculate the UB Matrix, you need to know lattice parameters and two reflections
- UB Matrix depends on the orientation of the crystal with respect to the instrument (Eulerian cradle)



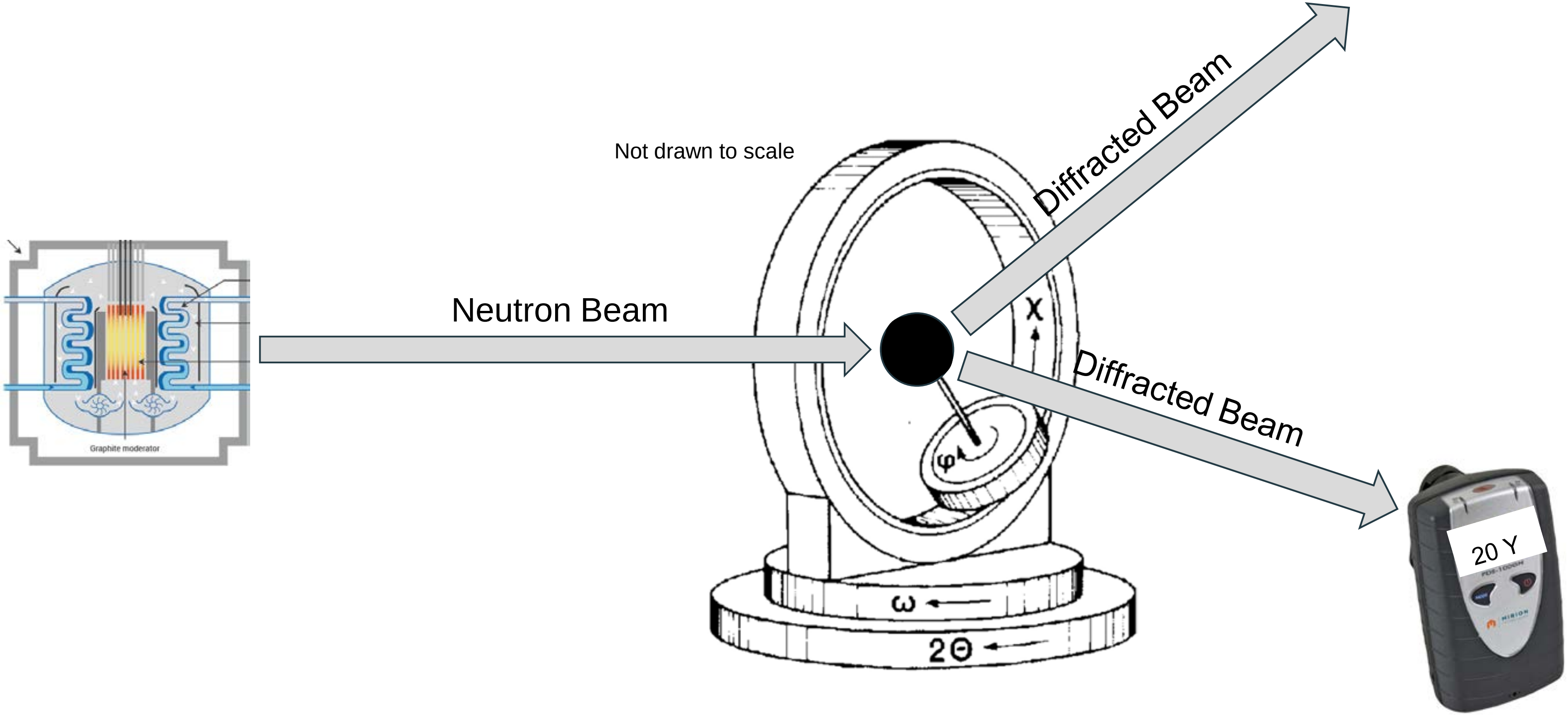
UB Matrix



CHI-PHI SPACE
HKL SPACE
PHI (degrees)
70
60
50
40
30
20
10
0
0
10
20
30
40
CHI (degrees)
(0k0)
1
0
0
0.2
0.4
0.6
0.8
1
1.2
(h00)

Current Methods

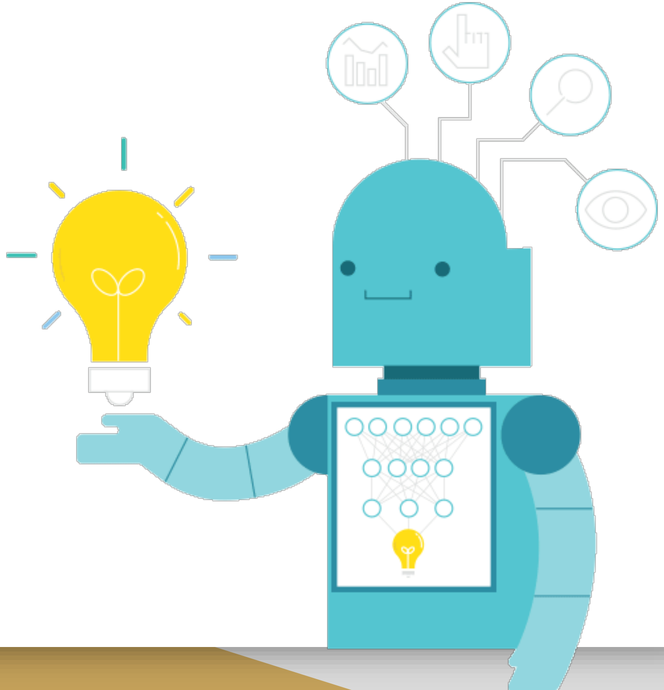
- Set the crystal in Eulerian cradle
- Rotate “randomly” until a reflection is hit
- Assume where other reflections might be and search this area until a reflection is hit
- Once a sufficient amount of reflections are hit, the UB matrix can be created
- Tedious, time consuming, and requires attention



Not drawn to scale
Neutron Beam
Diffracted Beam
Diffracted Beam
Graphite moderator
χ
φ
ω
2Θ
20 Y

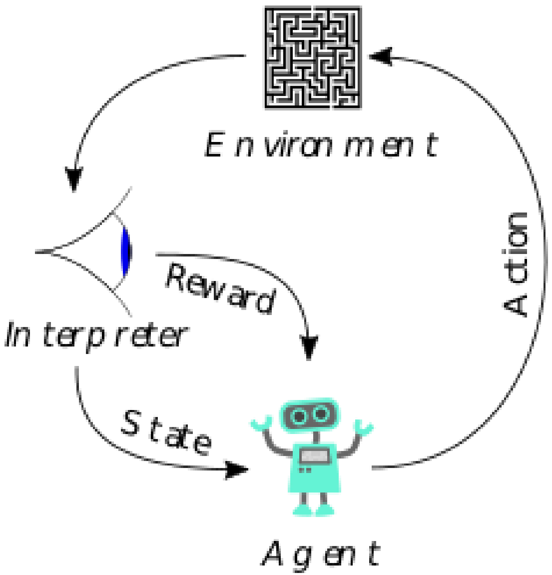
The Solution (Hopefully)

- Automate the alignment process using machine learning
- Find the fastest and most efficient way to find reflections
- Make the process universal for all crystals, regardless of symmetry



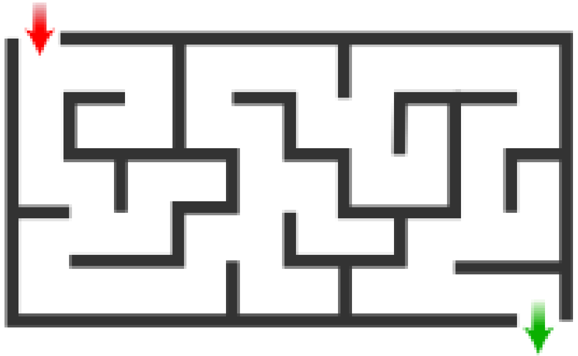
Reinforcement Learning

- ➢ We can simulate the crystal and the instrument in a program
- ➢ If the crystal is moved to a diffracting position for a specific 2Θ:
  - Give the agent a reward (reinforcement)
  - The faster it gets there the more the reward
  - Punish the agent by associating every move with a cost
- ➢ The agent will eventually be able to learn the fastest way to get into a diffracting position
  - Tensorflow



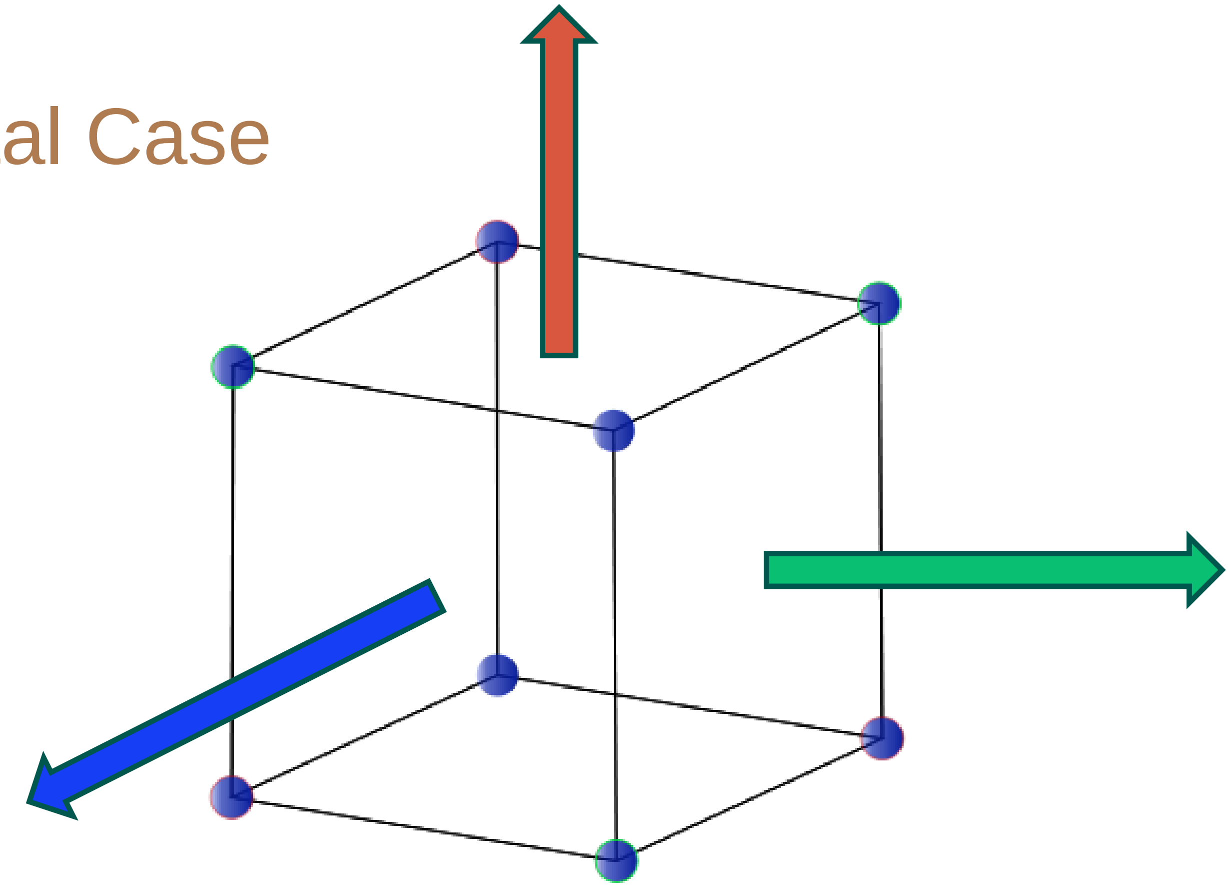
Epsilon-Greedy

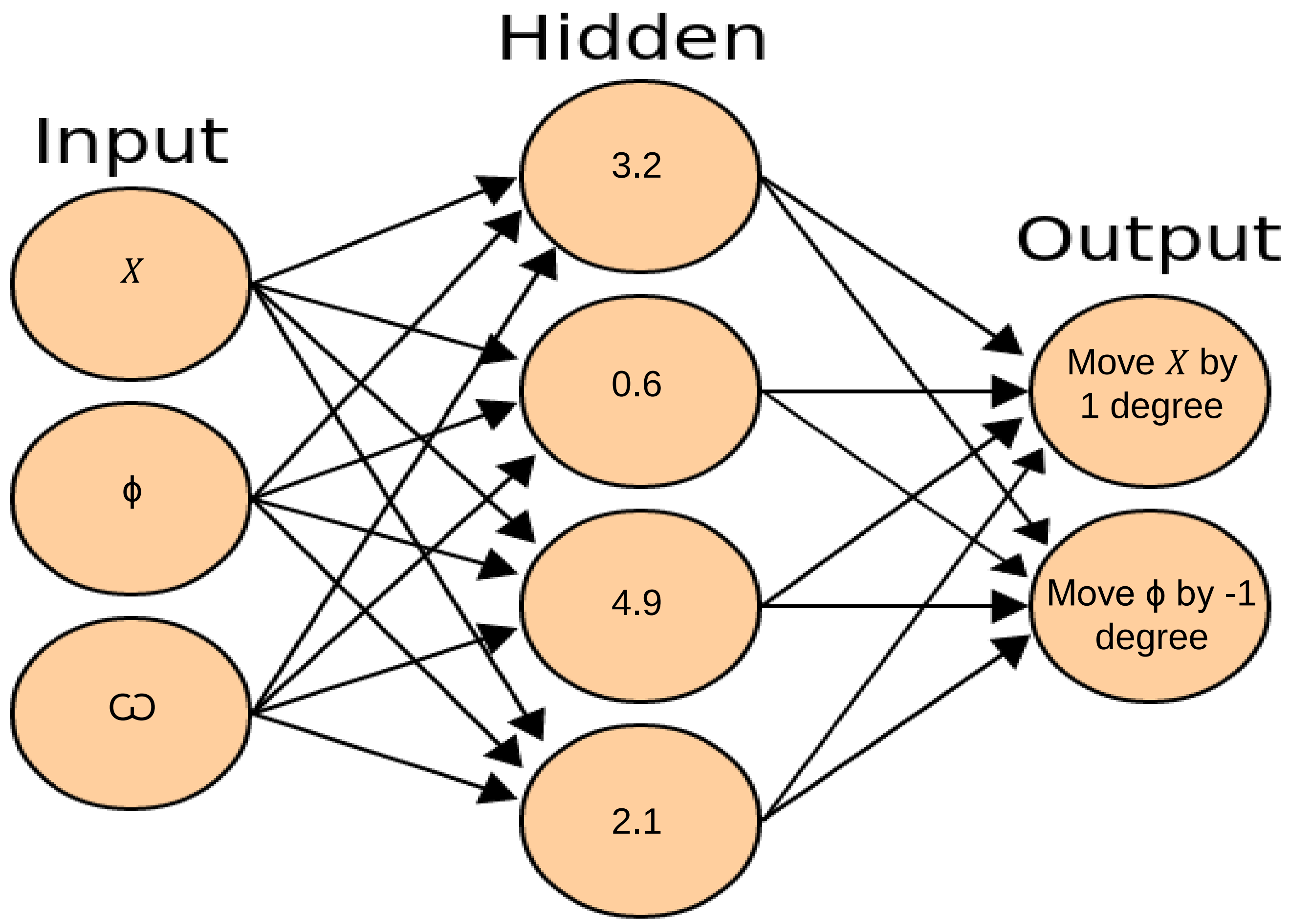
- Once a reflection is hit, continue using this method as our go-to
- Every now and then, make a random move
- If the move results in less reward, don't make that move again
- If the move results in more reward, this new path becomes our go-to
- Repeat



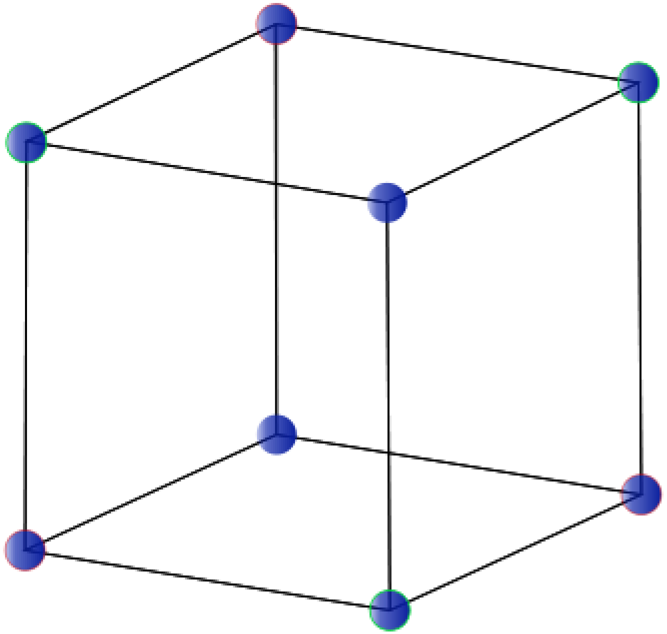
Reflection

Crystal Case

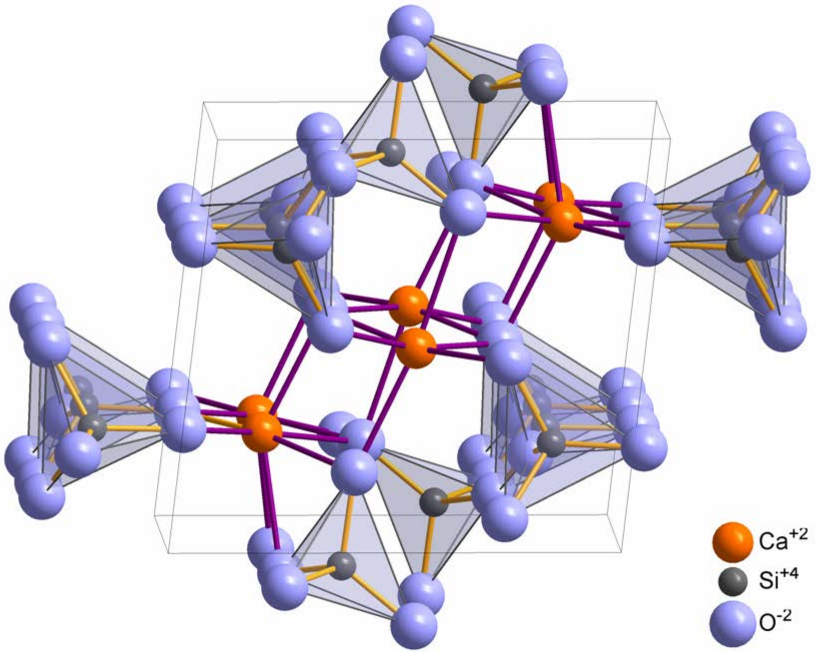



Hidden
Input
Output
X
ϕ
ω
3.2
0.6
4.9
2.1
Move X by 1 degree
Move ϕ by -1 degree

General Case



Triclinic Wollastonite



Results

- Unfortunately, the simulations were unable to find reflections in a respectable time
- Advantages of automation are belittled by the amount of time needed
- Difference between learning to find a point and learning how to find a point
- More work to be done in order to take advantage of this technique

Acknowledgements ☺

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Any Questions?