Automating the Alignment of Crystals

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Background

- The structure of crystals help scientists understand its properties.
- Crystal must be aligned to determine its orientation.
- These features can be hard to find for various reasons.
- Strontium Titanate ($\text{SrTiO}_3$), for example:
  - Simple cubic geometry
  - Obtains a large dielectric constant at cold temperatures
  - Becomes a superconductor at 0.35 K
Neutron Beam

\[ 2d \sin \theta = n \lambda \]
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 (χ), 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 ($X, \phi, \psi, 2\Theta$) 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

CHI (degrees)

PHI (degrees)

(h00)

(0k0)
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
The Solution

- 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 $2\theta$:
  - 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
Move $X$ by $1$ degree

Move $\phi$ by $-1$ degree
General Case

Triclinic Wollastonite

- Ca$^{+2}$
- Si$^{+4}$
- O$^{-2}$
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
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Any Questions?