pyXRD

- in this file I will present how it works -

This is a package made to calculate the XRD peofile giving the structuree, and also to plot it.

To calculate the XRD we must do 2 things

1. Calculate peak positions

C possible giving { - unit cell params (a, b, c, α, β, γ)
- wavelenght of XRay used (in Å)

2. Calculate Structuree Factors

C possible giving { - Atoms present
- Atoms positions
- Symmetry Geoup
- peak position (angles and hkls)
- a_i, b_i, c_i coefficients (in literatuee)

Bellow I will explain how I do these 2 things

- Calculate peak positions -

As known by the Beagg's low

$$\sin\theta_{hkl} = \frac{\lambda}{2 \cdot d_{hkl}}$$

if we know the wavenght of the Souece (λ) and the intee plavae distance (d_{hkl}) we can calculate the peak foe each plove (θ_{hkl}).

And if we define a plave h, k, l we can calculate it's d_{hkl} by calculating it's norm in the Reciprocal space ($|G_{hkl}|^2$) using the Relation

$$d_{hkl} = \frac{1}{|G_{hkl}|}$$

where

$$\vec{G}_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

unit cell vectors

$$\begin{cases} \vec{a}^* = \dfrac{\vec{b}\times\vec{c}}{V} \\ \vec{b}^* = \dfrac{\vec{c}\times\vec{a}}{V} \\ \vec{c}^* = \dfrac{\vec{a}\times\vec{b}}{V} \end{cases}, \quad V = \vec{a}\cdot(\vec{b}\times\vec{c})$$

So if I can pass theought all possible h, k, l I can calculate each peak position by just calculating

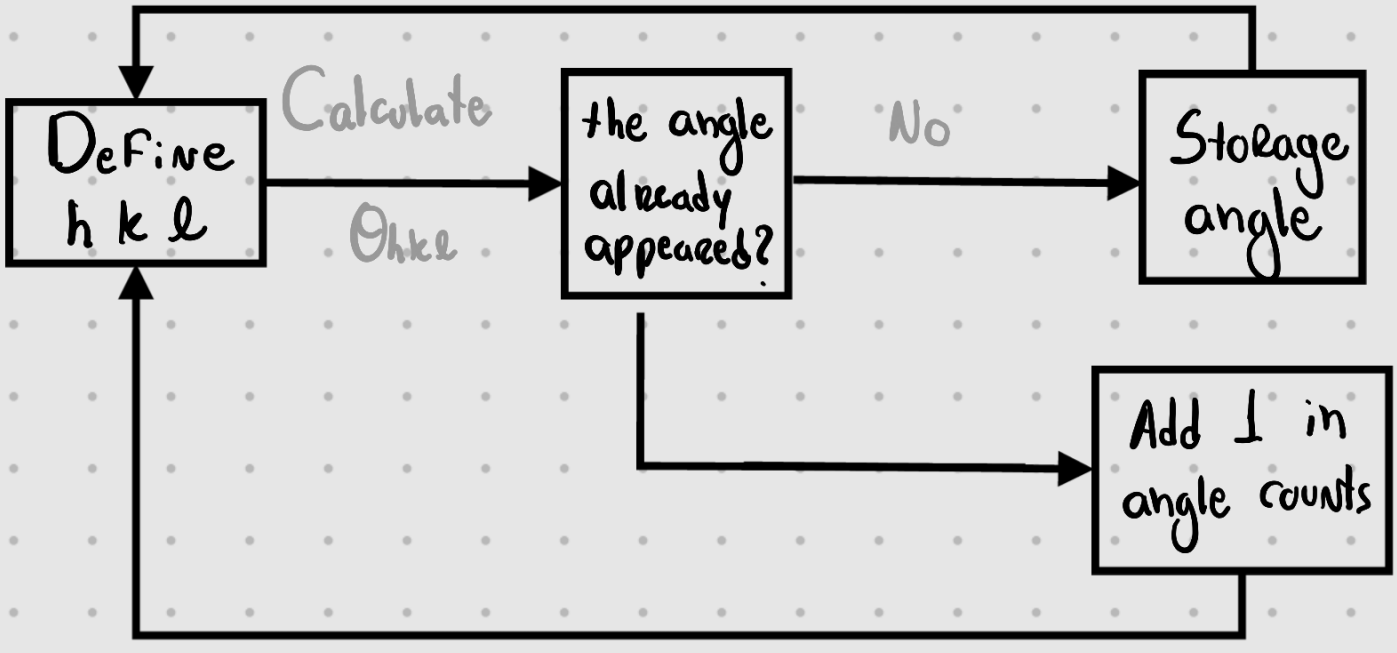
$$\theta_{hkl} = \arcsin\left(\frac{\lambda G}{2}\right)$$

But when doing it we must dischart planes that give the same angle (But save how many times one appear to use Futurally as a correction parameter.)

So I created a function

"generate_hkls" (implemented in Numba)

Where we follow the Flux.



Do this until we passed throught all possible hkls

I tend to inform a max value like 10 and we walk from -10 to 10 in h, k and l, so we have 3 loops one foe each index.

↖ (SLOWER PART OF CODE)

- Calculate Structure Factors -

The structure factors are defined for each plane

$$F_{(hkl)} = \sum_{j=1}^{N} f_j(hkl) \cdot e^{2\pi i \, \vec{r}_j \cdot \vec{G}_{hkl}},$$

where we sum over all the **primit**ive **u**nit **cell** atom positions ($\vec{r}_j$). Each atom having a atomic form factor ($f_j(hkl)$) depending on the atom element and calculated by

$$f_j(hkl) = \sum_{n=1}^{4} a_n \cdot e^{-b_n \cdot \left(\frac{\sin\theta_{hkl}}{\lambda}\right)^2} + C,$$

where the a_n, b_n and C constants are well defined.

Calculated for each atom by the function

`fhlk2`

As the norm of the structure factor is proportional to the intensity of each peak, so

$$I_{hkl} = |F_{hkl}|^2 \cdot L_p \cdot p$$

L_p: Correction term

p: multiplicity of each hkl (Calculated in "generate_hkl")

So we can create a function

"F_{hkl} B^T ϕ_{hkl}"

Where giving each hkl (θ_{hkl}) we calculate the intensity by suming over all atom position (in cartesion coordinates).

To obtain the primitive unit cell (define all atom positions used) I defined the function

"find_atoms_unit_cell"

which giving the wyckoff positions the symmetries are applied.