**Guidance for 2D-XRD Modelling**

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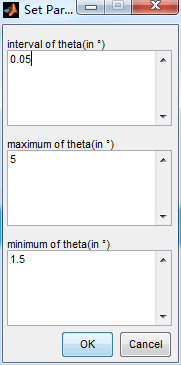
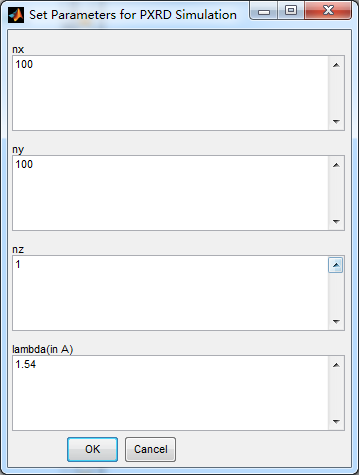
This guidance is for 2D-XRD-Modelling, which aims to simulate PXRD (Powder X-ray Diffraction) patterns of 2D materials with finite size in matlab. The basic theoretical method is a complete integrating method in real space (CIREAL). This code uses the published Numerical Integration Toolbox in matlab. Depending on the parameters and simulated crystal structures, the calculated time can be from several minutes to several hours.

1. **Preparing Crystal Structures**

The first step for simulation is to read in a crystal structure for simulation. This code read in one common structure file, ***cif***s, which should be exported by **Material Studio**, a common software for crystal structures. And the interlayer axis should also be set as axis c. It is recommended to read in a structure with **primary unit cell** because we simulated crystals with a size of nx\*ny\*nz, where all of them are integers. If the code read in a crystal structure with two layers in one unit cell, then the simulated is always conducted within the limitation that the layer number is always even, no matter what nz is.

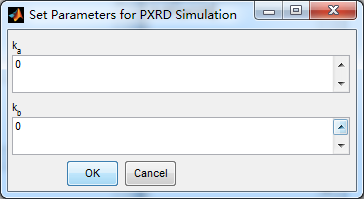
1. **Setting Parameters for Simulation**

After preparing the ***cif*** files, open ***MODELONE.m*** and run. One should set the size of simulated crystals, corresponding X-ray wavelength, and the diffraction angle range and corresponding angle interval through the following windows:



It’s is safe to set interval of theta not small enough because around the peak positions, the code will set a series of very small intervals to ensure not missing the peak positions.

Then two important parameters should be set, ka and kb. This two parameters describe the interlayer shifting vector’s weight on axis a and axis b. Which means the shifting vector axis c can be expresses as , where is vertical to the a-b plane.



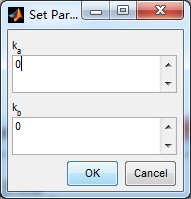
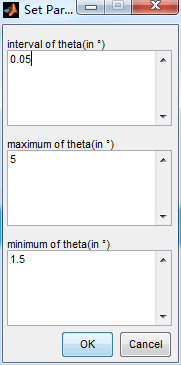
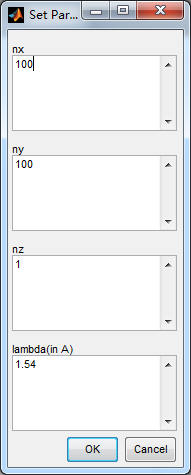
For simulation of crystals stacked in eclipsed model, we one simply set ka and kb as zero.

For simulation of crystals in staggered model, one should set ka and kb respectively.

1. **Examples for Eclipsed and Staggered Crystals**

Here we demonstrate two simulation process through a MOF, Zr-TCBPE by building the crystal structure in eclipsed model or staggered model. These two structure files can be found in the EXAMPLE file.

For the eclipsed model, we read in the structure file, ***2D Zr-TCBPE-eclipsed.cif*** , and it’s simple that we set parameters as following:

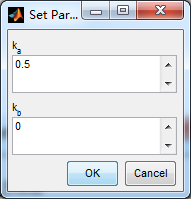
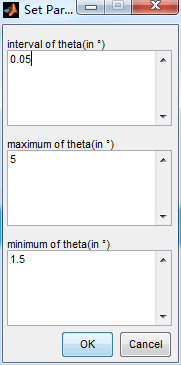
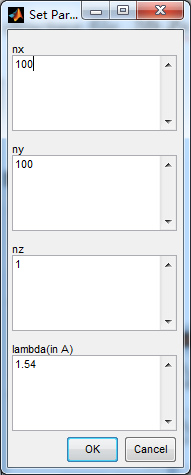


Then choice the file ***2D Zr-TCBPE-eclipsed.cif***.

Then we can get the result within minutes. One can change *nz* to see the relationship between PXRD patterns and layer number.

For the staggered model, we read in the structure file, ***2D Zr-TCBPE-staggered.cif*** , and in this structure we find the primary unit cell and build the interlayer axis as :

So the parameters should be set as :



Then we can get the result about one hour. One can change *nz* to see the relationship between PXRD patterns and layer number. Then choice the file ***2D Zr-TCBPE-staggered.cif***. After getting the result, we use Hermite interpolation to smooth the curve.