# Goal: Simulate (before refining if datasets are good enough) powder diffractograms of butanol during crystallisation/melting cycles.

We expect to see effects of:

- crystal shape from the nanoparticles
- possibly from stacking faults (2 possible stacking layers to be studied)

For the moment, testing the simulation on:

- crystallites shaped by (100), (010) & (001) faces and symmetry equivalent
- regular stacking of (001) layers (i.e. no defects) ➔ simulated crystallites look fine compared to normal 3D structure

in order to check if we can reproduce qualitatively the intensities of simulated data of ideal powder
(verification before going further into analyses)

**Problem encountered:**

The diffractograms simulated « altern » between 2 types depending of the size of the particle & the type of calculation performed. One is the expected diffractogram (main peak at 2theta~78°), the other one is totally different
with wrong intensities but peaks still at Bragg position (next slides).
These are reproduced for:

- different crystallite sizes
- calculation options in the powder module:
  - ✓ Calc = comp or debye
  - ✓ Four = four, stack, normal (I don't know what is « normal » mode, I've pasted it from one of the examples)

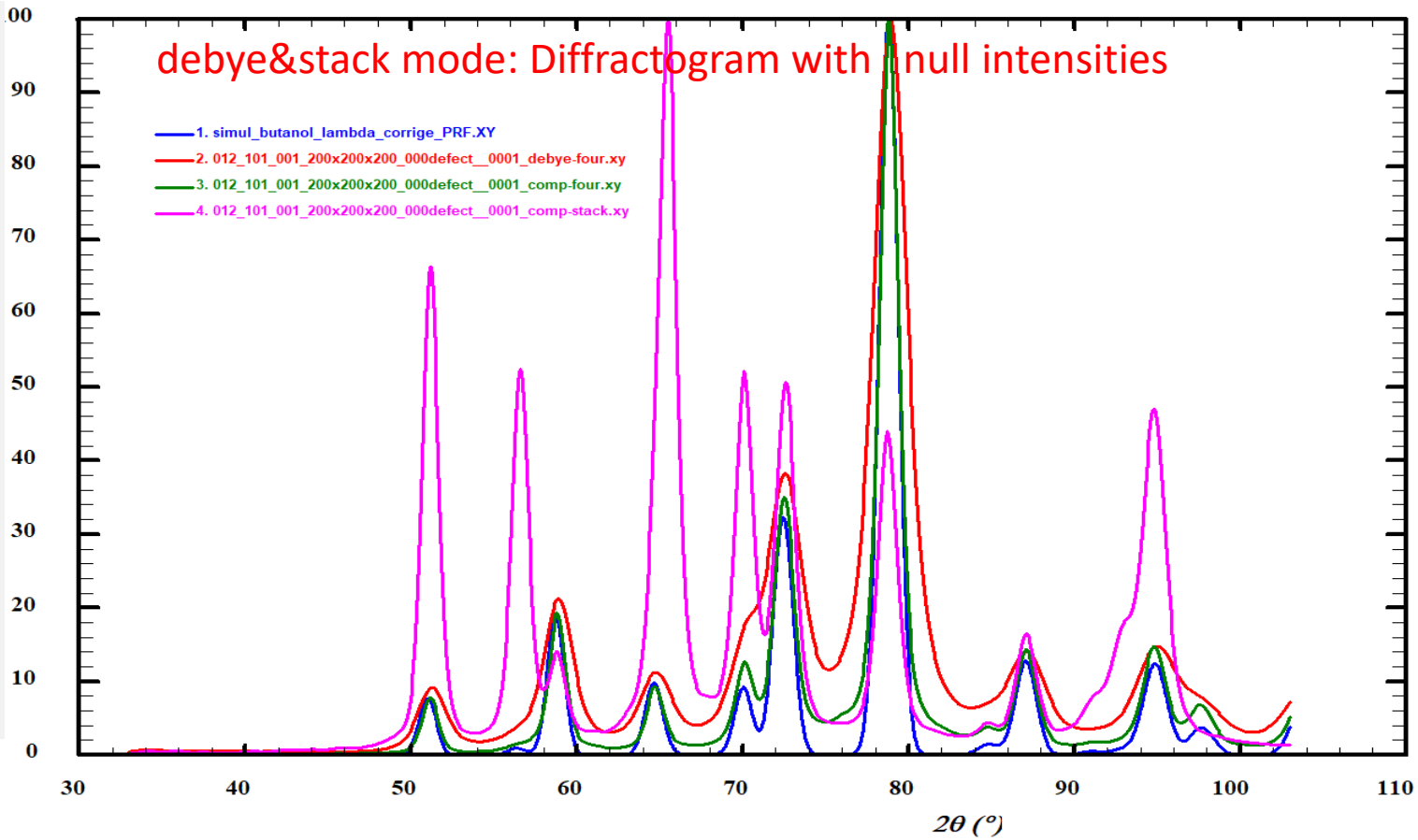
# Testing calculation modes for diffractograms :

## Crystallite without fault generated by a stacking of (001) layers: (100)x(010)x(001) = 200x200x200 Å

In the « powder.mac » module, 2 x 2 modes tested
set calc, debye // complete
set four, four // stack (“normal” tested afterward)

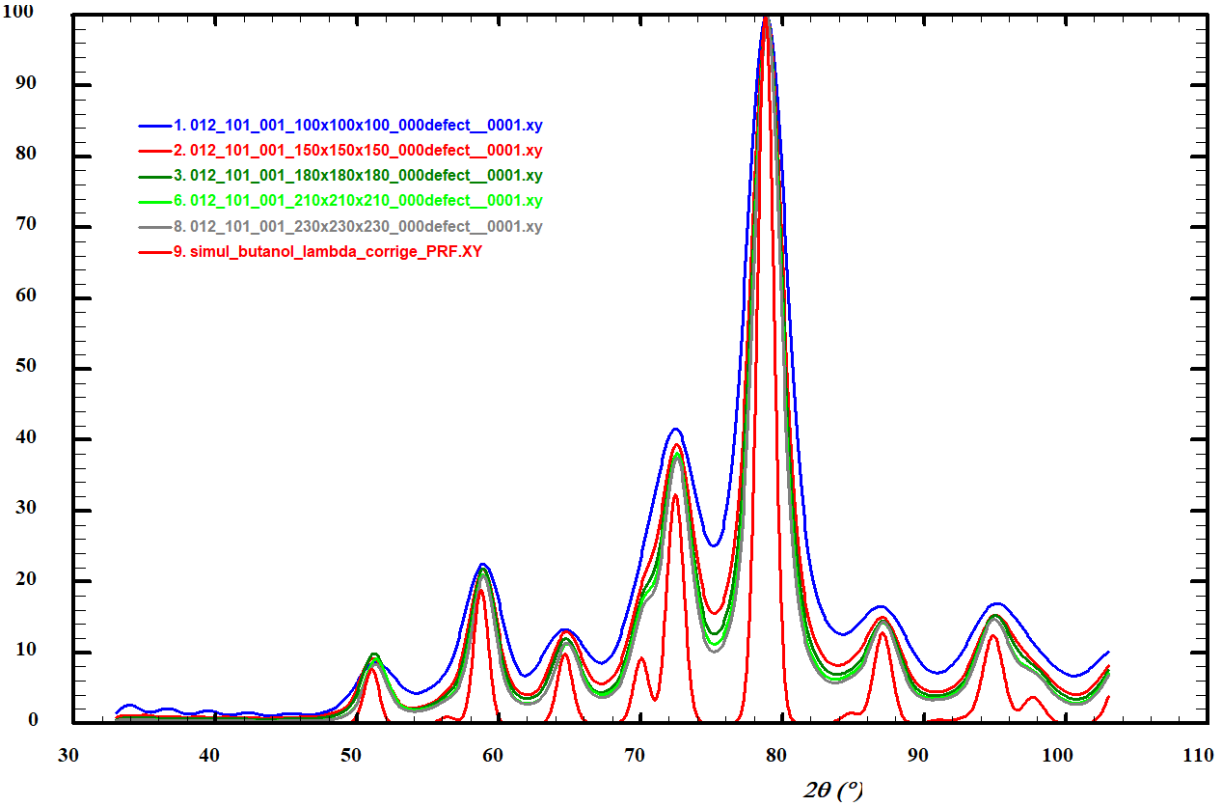
| Four/Calc | debye | complete |
|---|---|---|
| four | 3235 s | 261 s |
| stack | 3275 s<br>**Intensité=0** | 463 s |

```
powder
  neut
  set axis,tth
  set calc,debye
  set disp,off
  set delta,0.0
  set tthmin,33.0
  set tthmax,103.0
  set dtth,  0.1
  set temp,use
  set four,four
  set lpcor,neutron
  set wvle,4.632871
  set profile, pseudo
  set profile,uvw,3.042,-2.295,1.639
run
exit
```

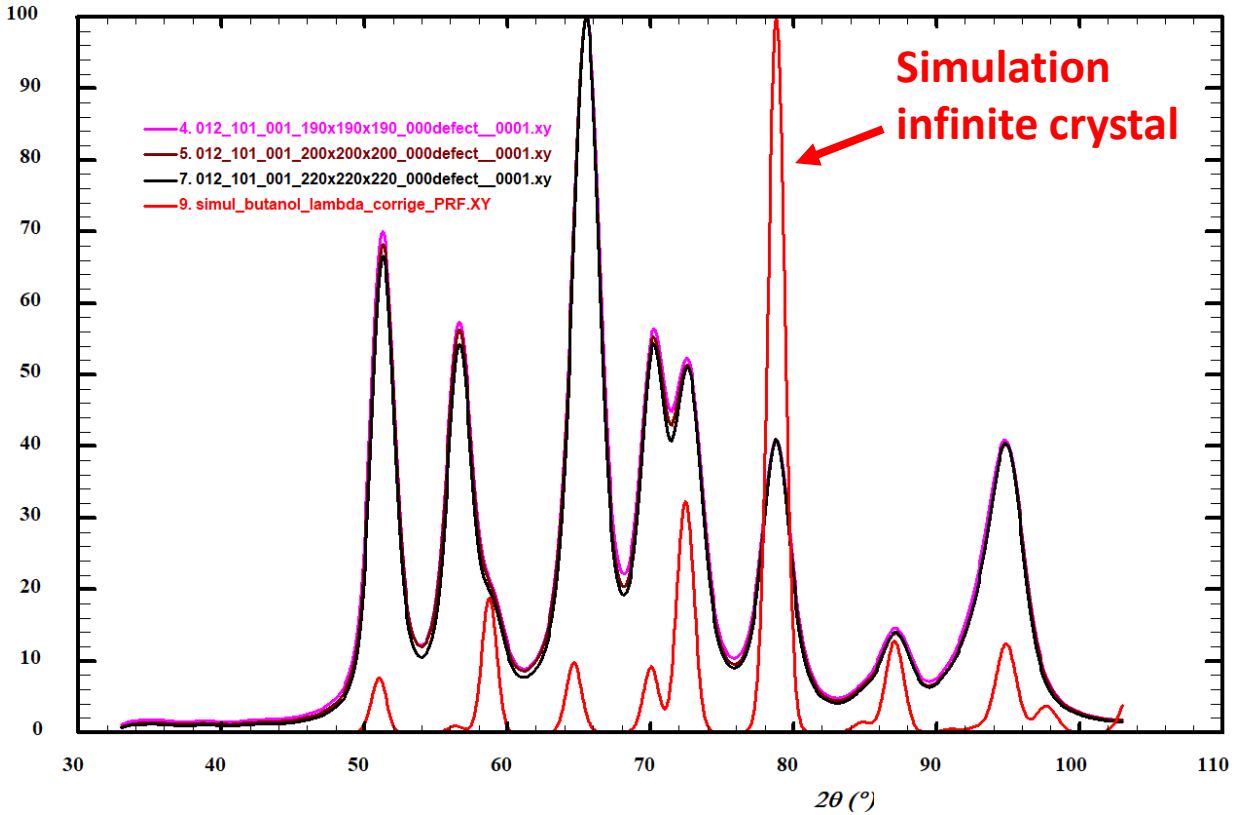


# Testing calculation modes for diffractograms :

Crystallite without fault generated by a stacking of (001) layers: (100)x(010)x(001): **Debye & Four mode**



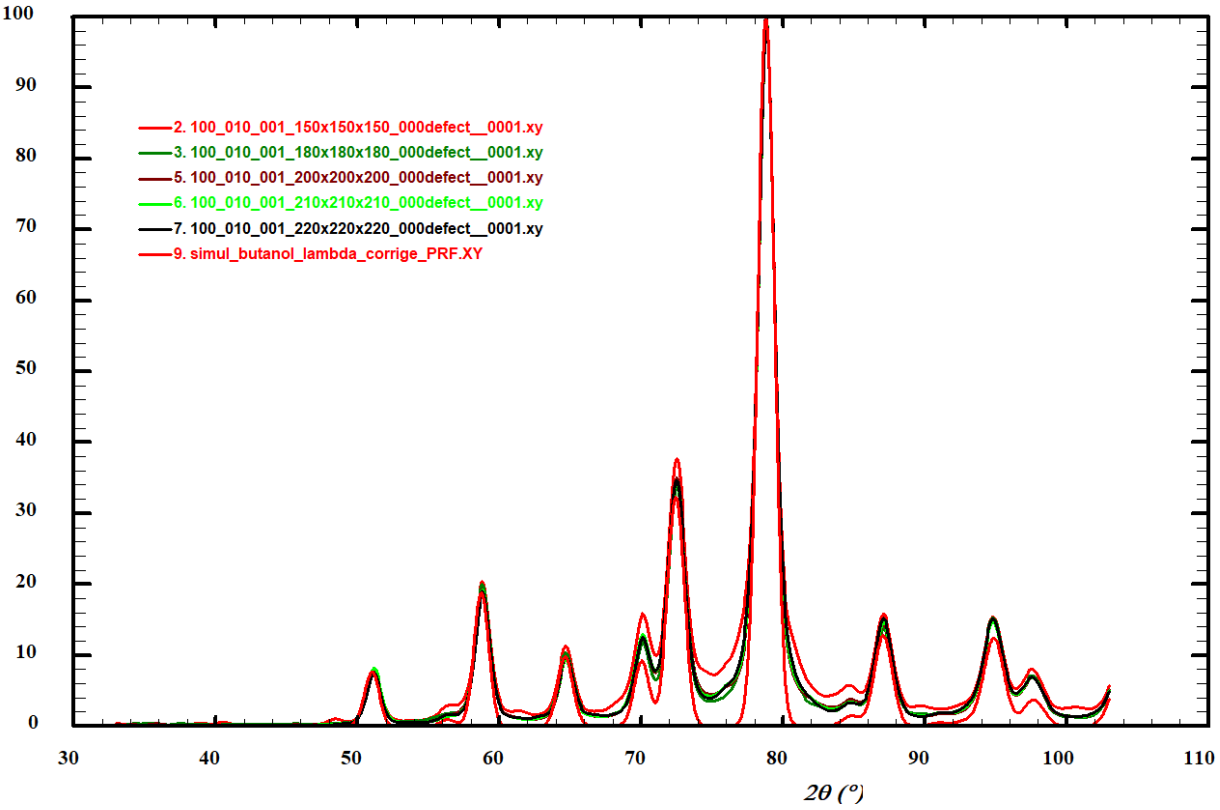

Diffractogram (100)x(010)x(001) **OK** for sizes:
100, 150, 180, 210, 230



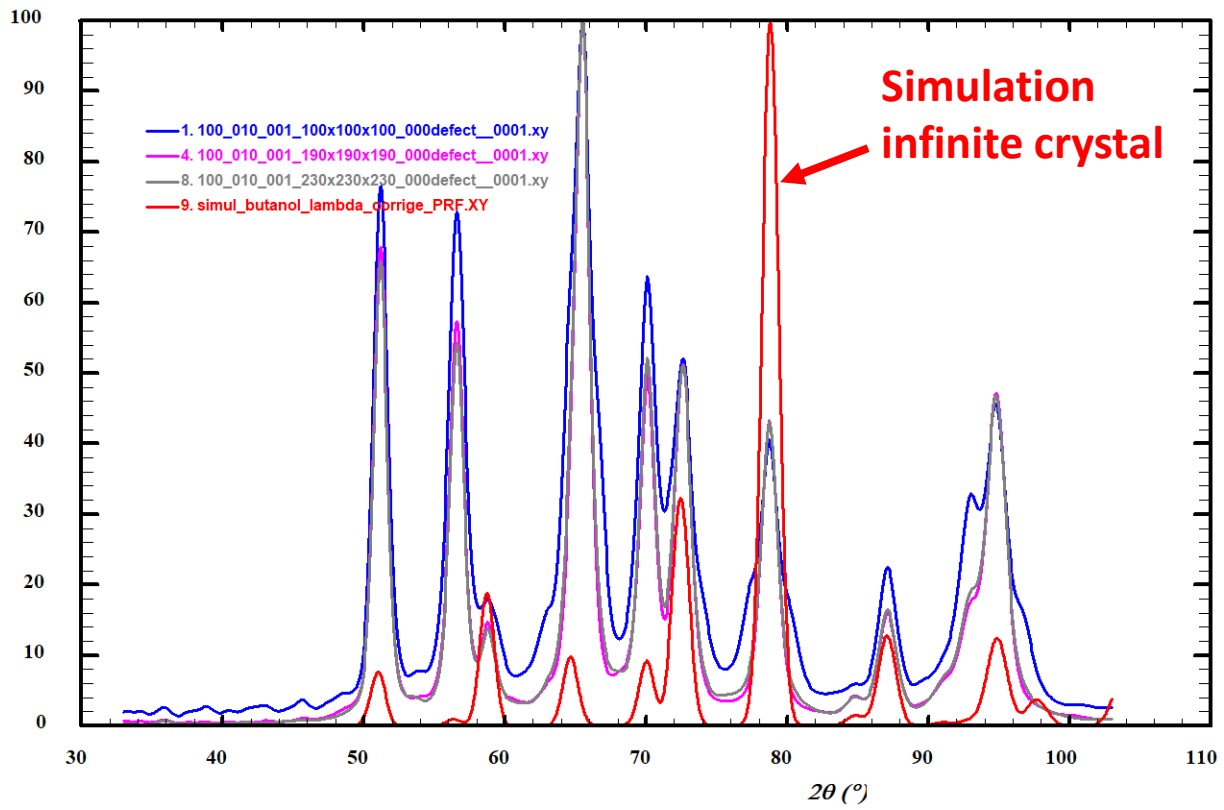

Diffractogram (100)x(010)x(001) **bad** for sizes:
190, 200, 220

# Testing calculation modes for diffractograms :

Crystallite without fault generated by a stacking of (001) layers: (100)x(010)x(001): **Comp & Four mode**



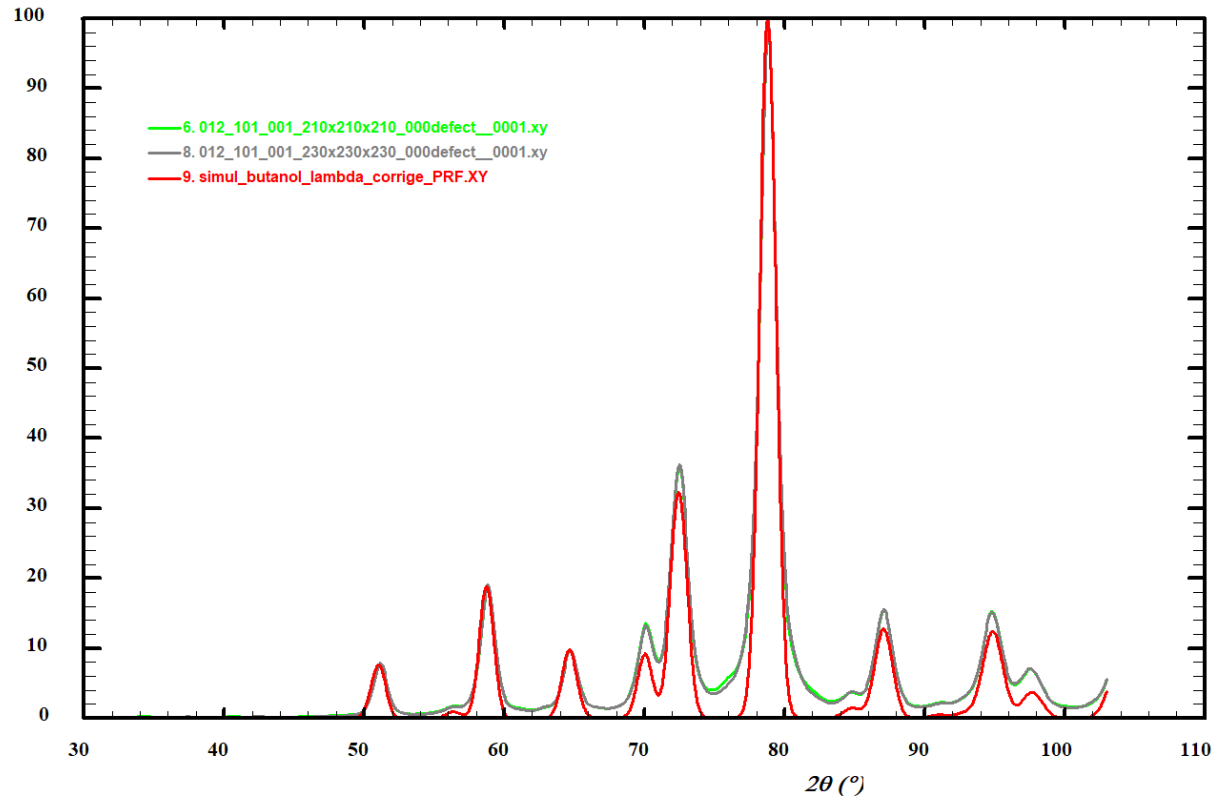

Diffractogram (100)x(010)x(001) OK for sizes:
150, 180, 200, 210, 220

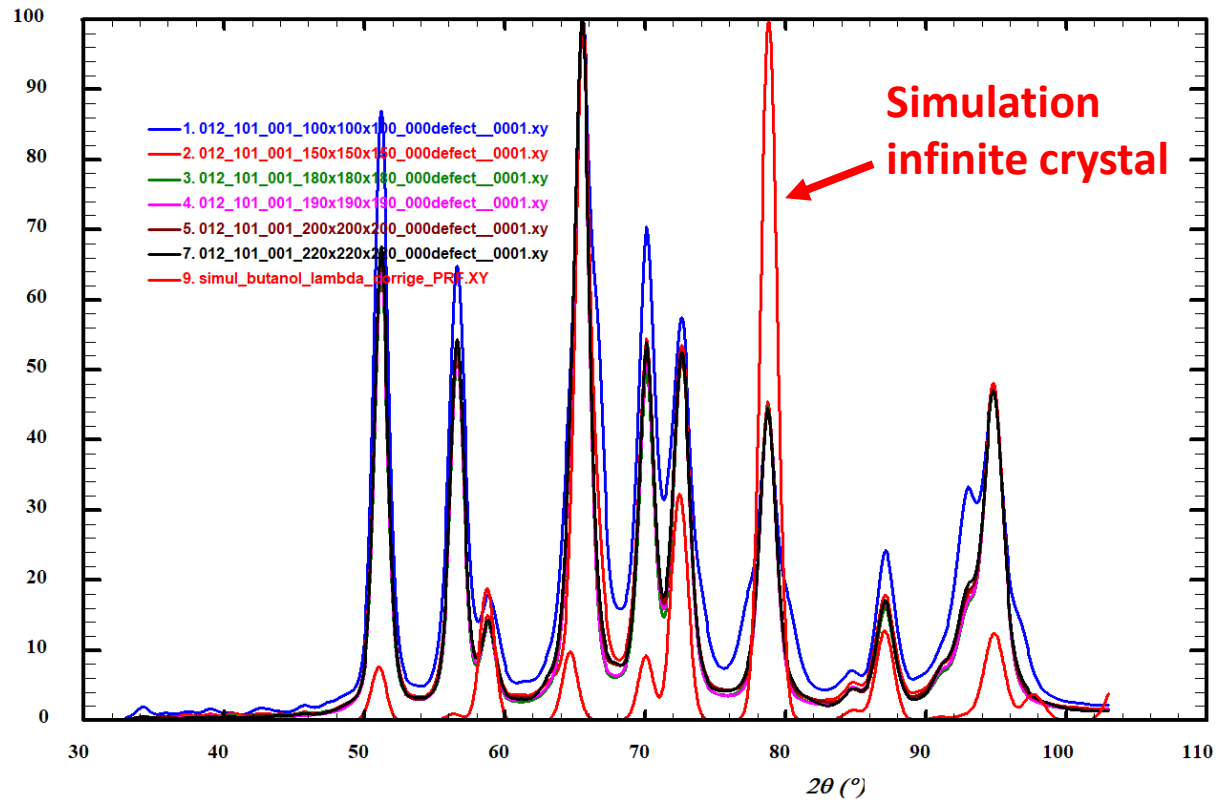



Diffractogram (100)x(010)x(001) bad for sizes:
100, 190, 230

# Testing calculation modes for diffractograms :

Crystallite without fault generated by a stacking of (001) layers: (100)x(010)x(001): **Comp & Stack mode**



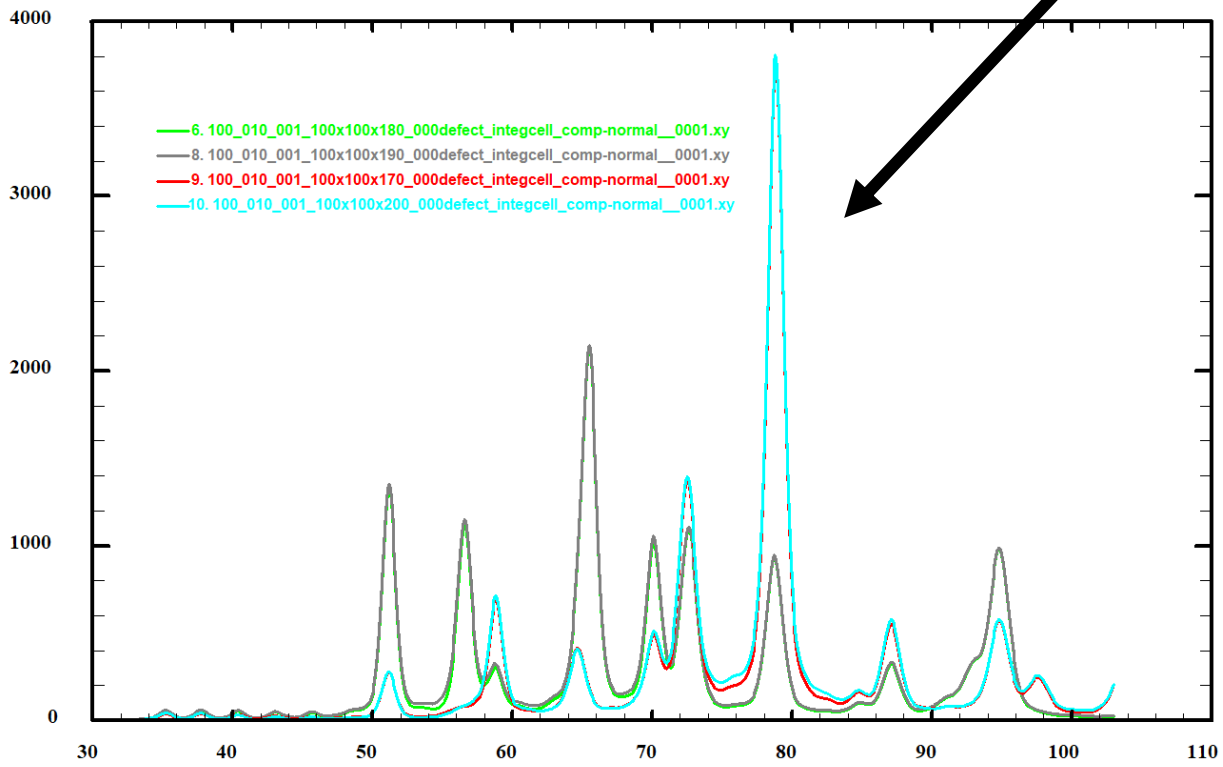

Diffractogram (100)x(010)x(001) OK for sizes:
210, 230

Diffractogram (100)x(010)x(001) bad for sizes:
100, 150, 180, 190, 200, 220

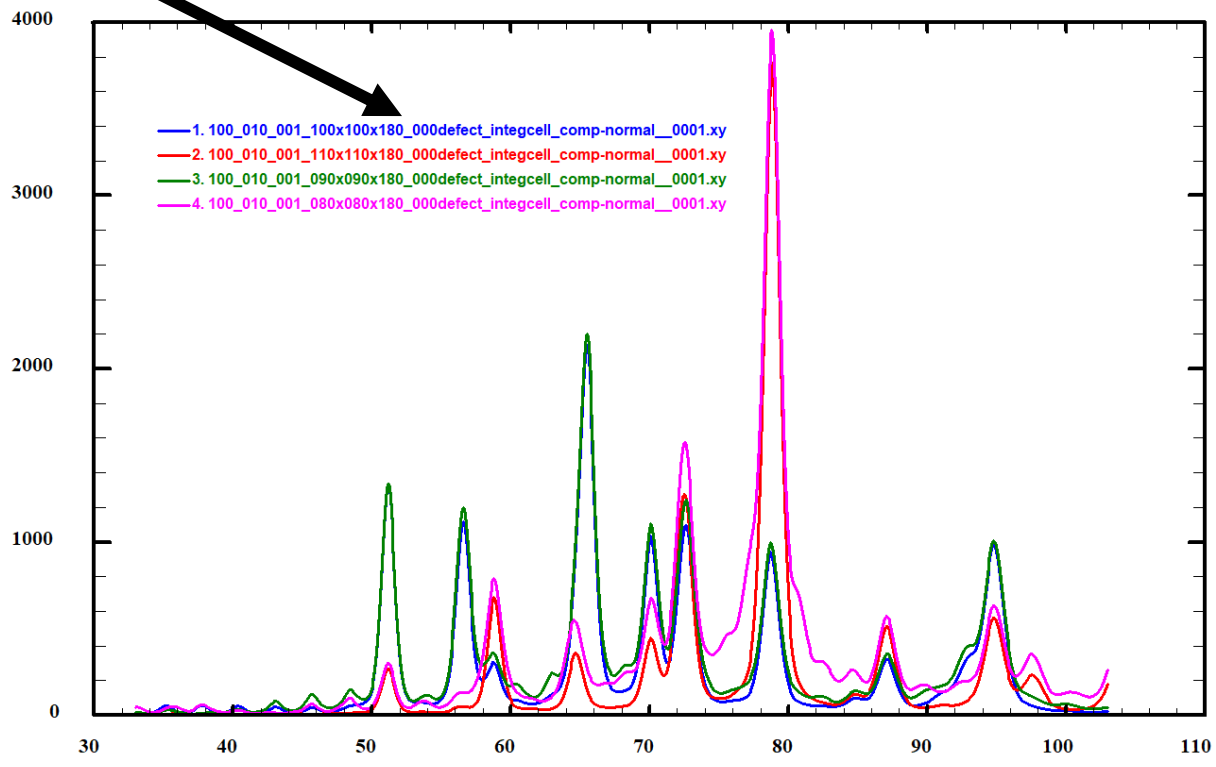
**Modifications tested:**

- Crystallite size set with the command « boundary » inside the « surface » sub-menu instead of main discus level
- Crystallite size set from integer number of crystal cells or round number in angstroem

➔ Problem still there but for other sizes… (001) size & (100)/(010) size have similar effect




*(100)x(010) sizes = ~100x100Å (integer number of cells)*
*(001) Size varying*




*(001) size = ~180Å (integer number of cell)*
*(100)x(010) Sizes varying*