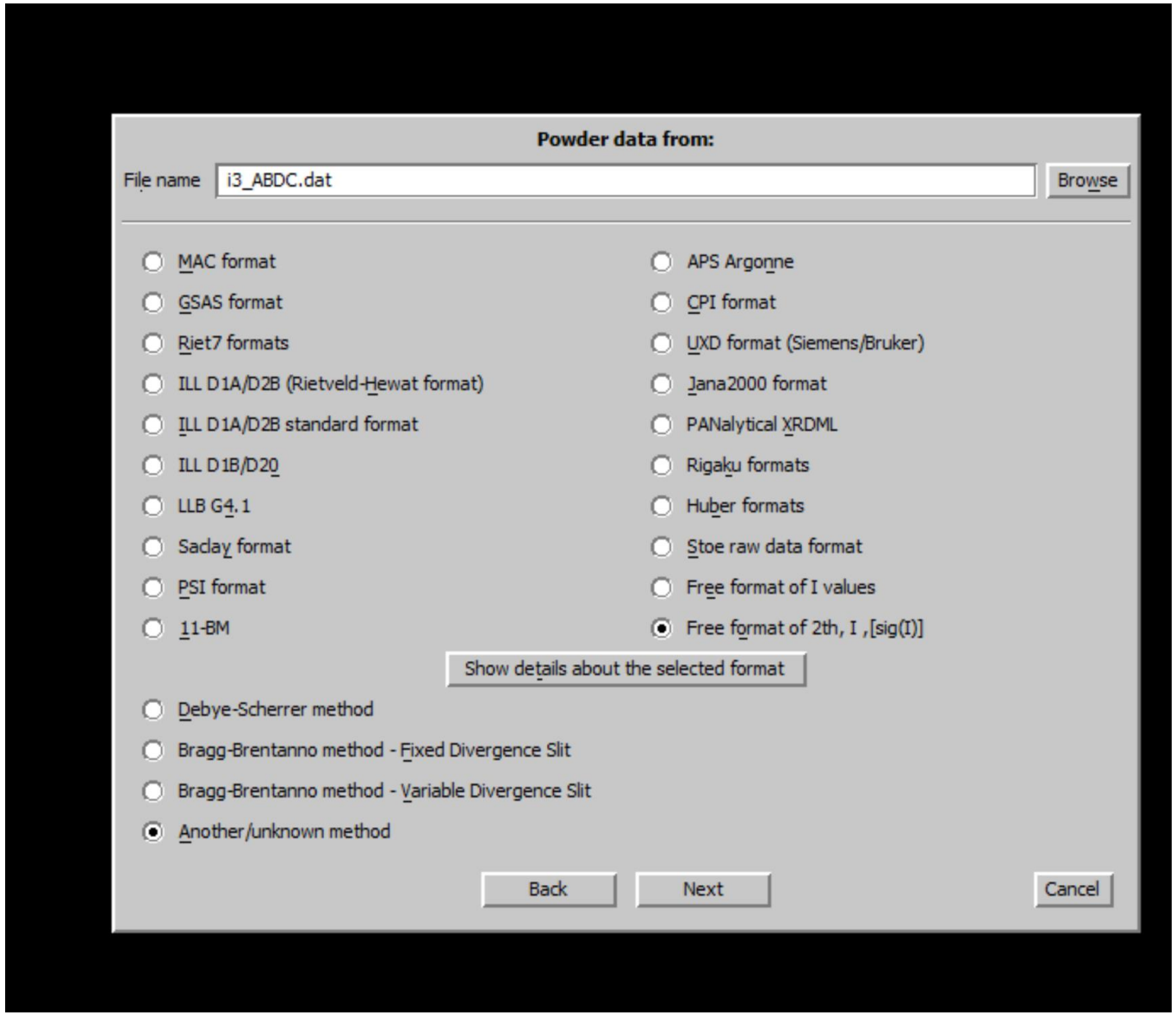
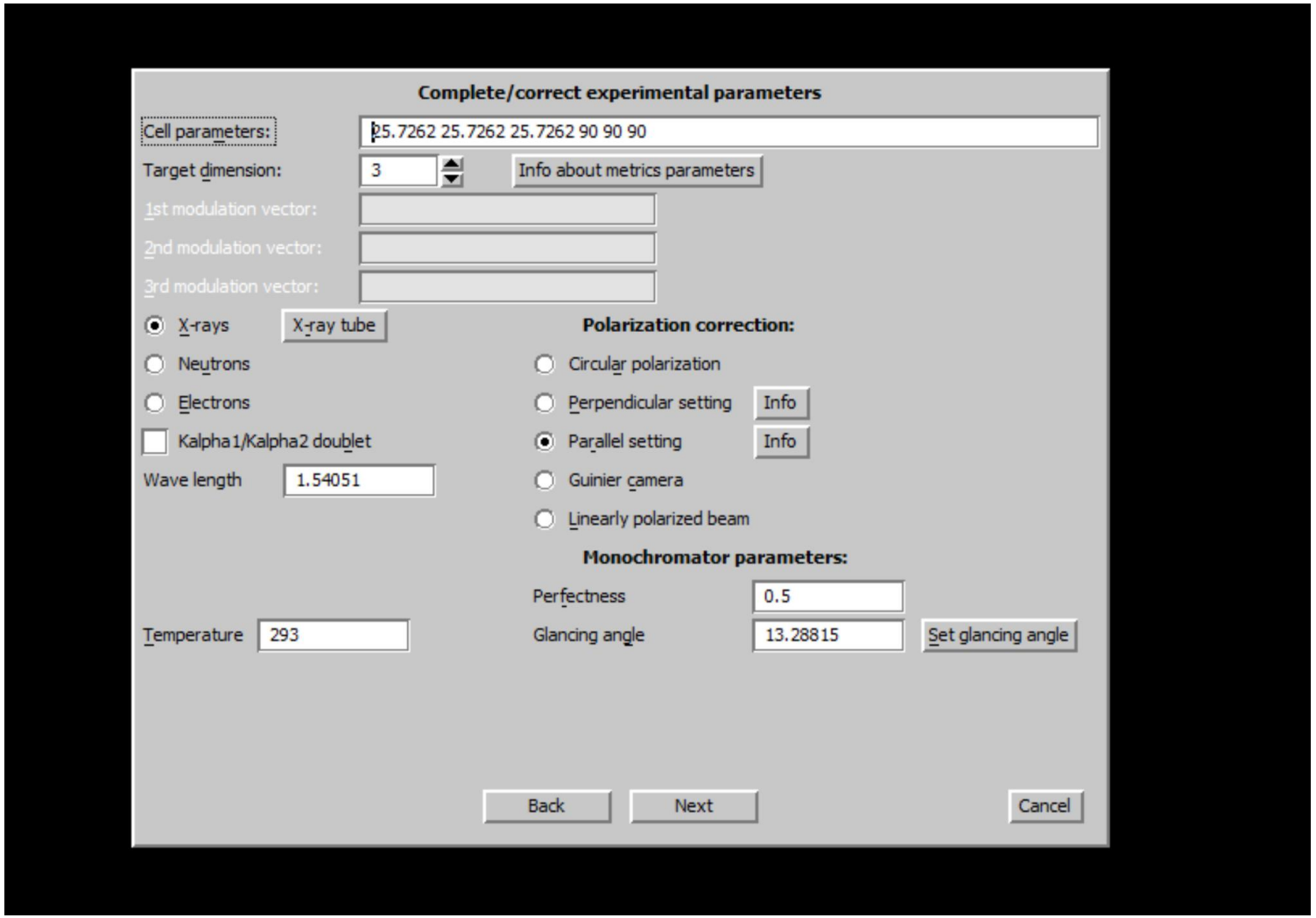
Basic Powder X-ray Diffraction Analysis

Import your data files



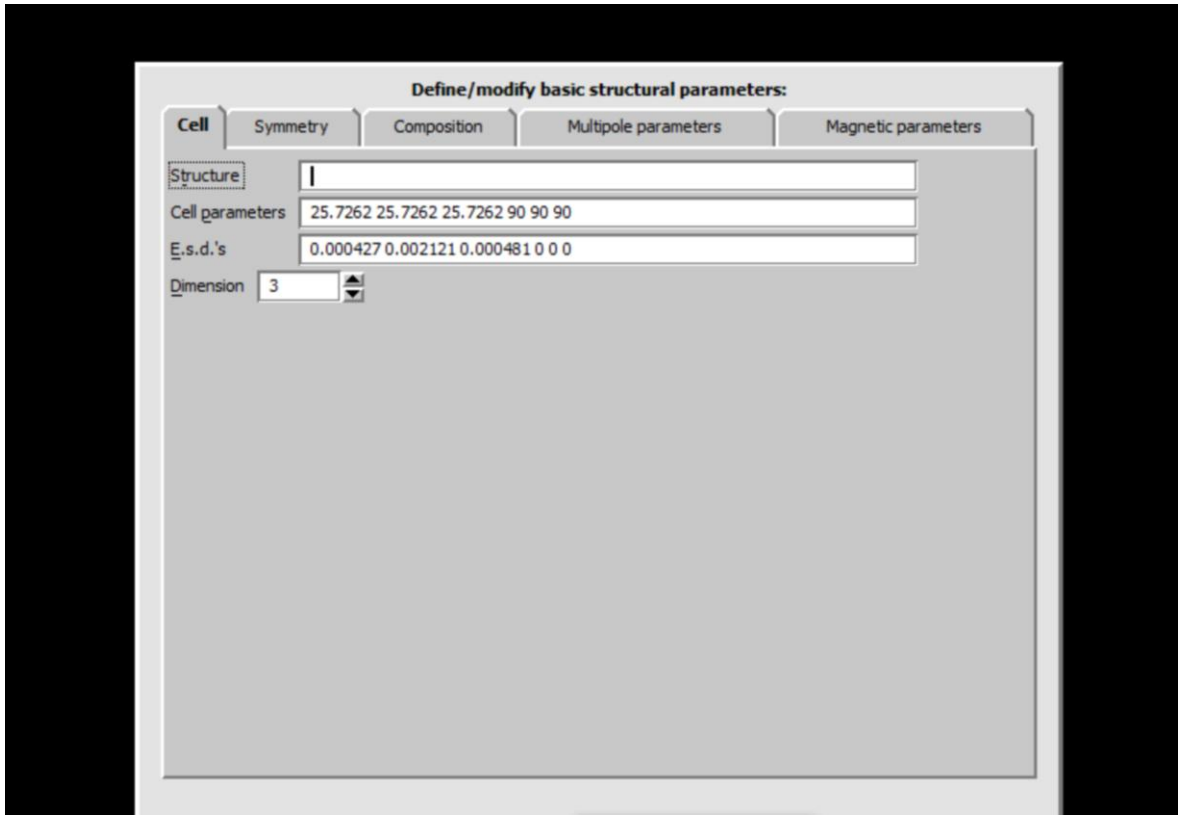
Important!
Rename your .xyd file to .dat

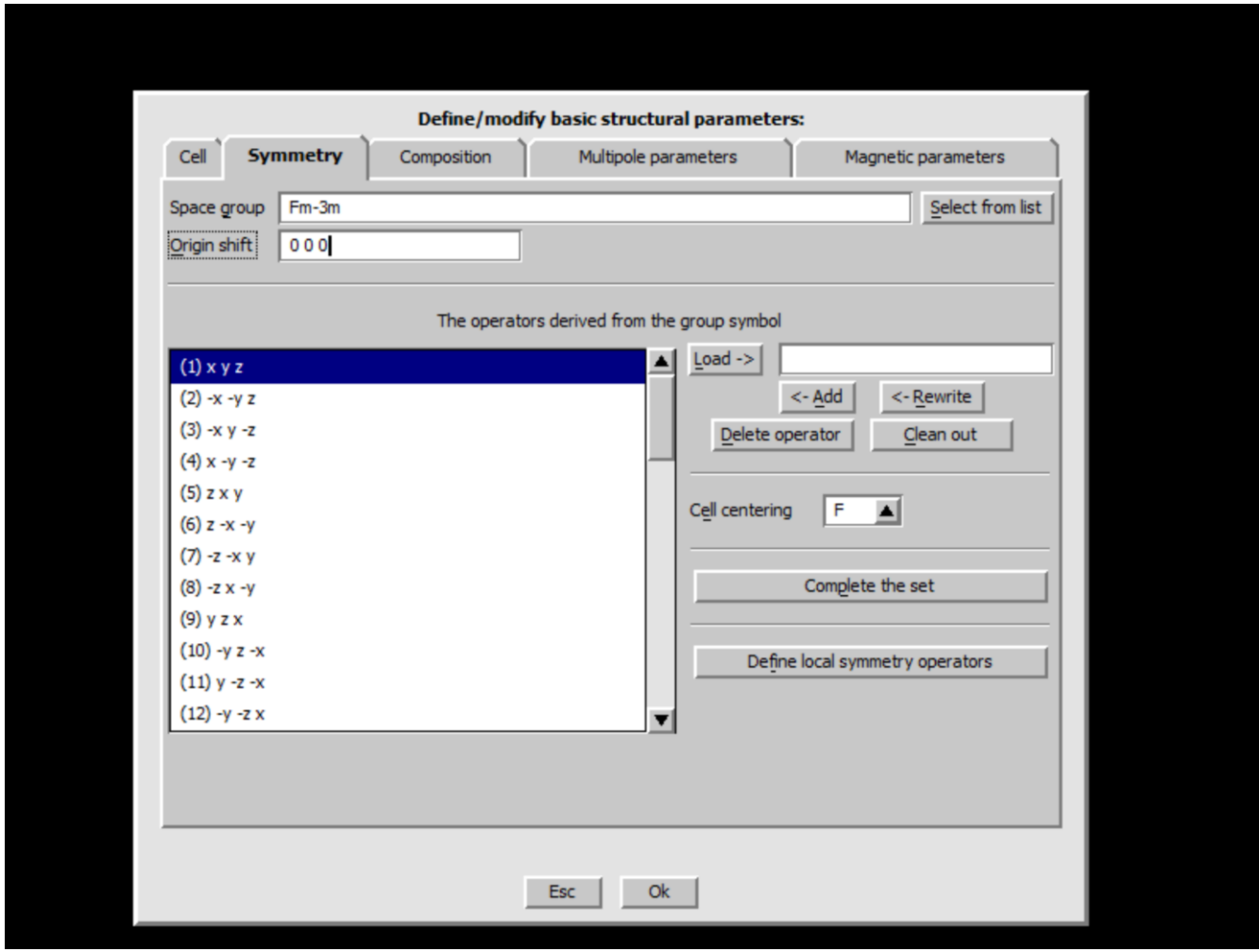
Input your “guessed” lattice parameters



Edit your M50 file

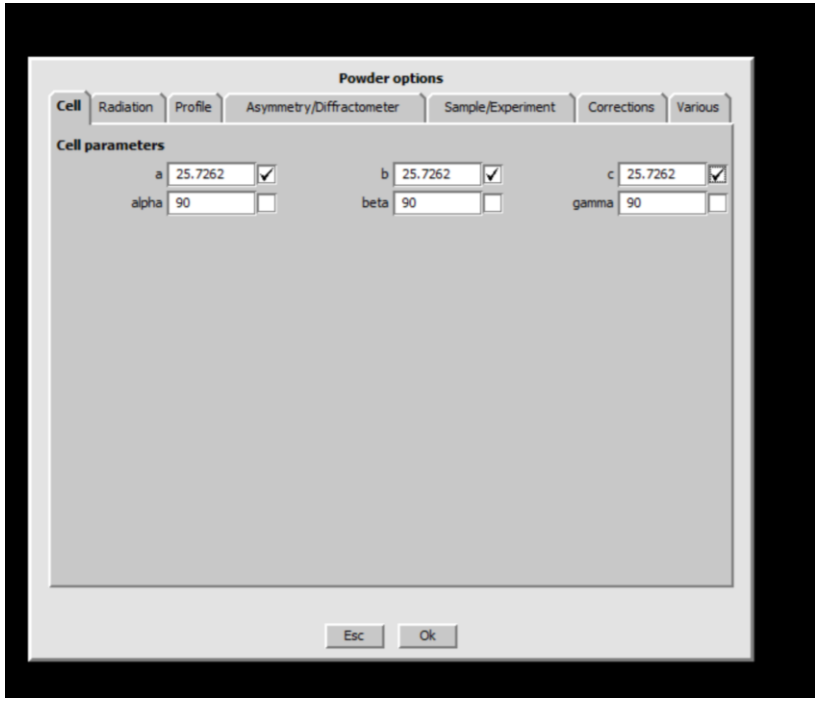
Important!
Change the space group to the one from the .cif file



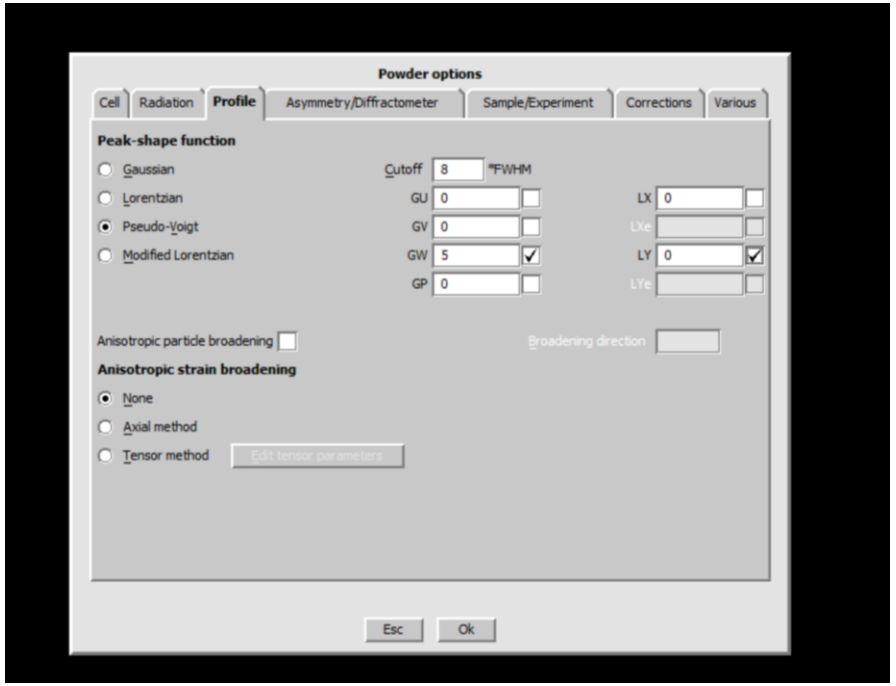


Edit your powder diffraction profile

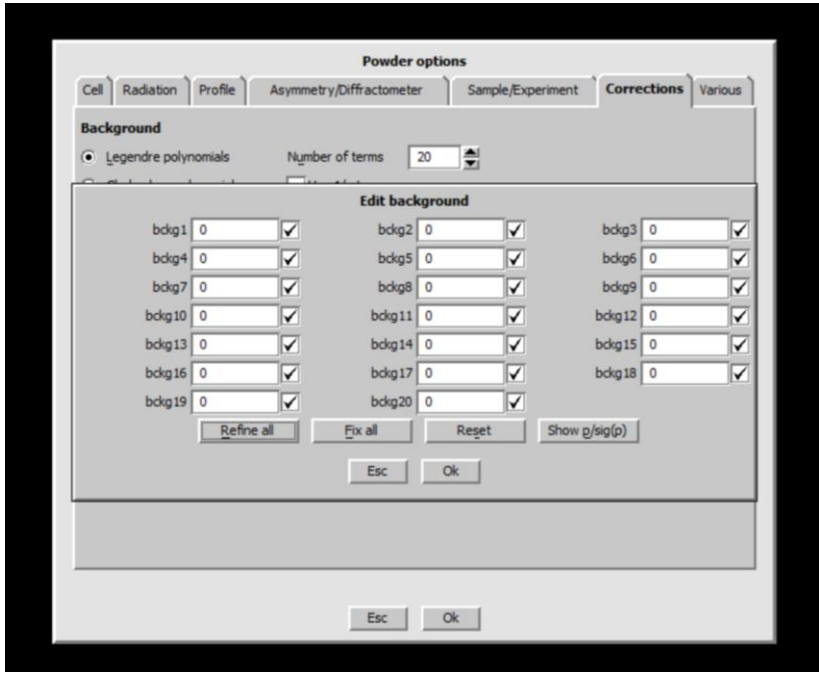
Important!
Refine your lattice parameters



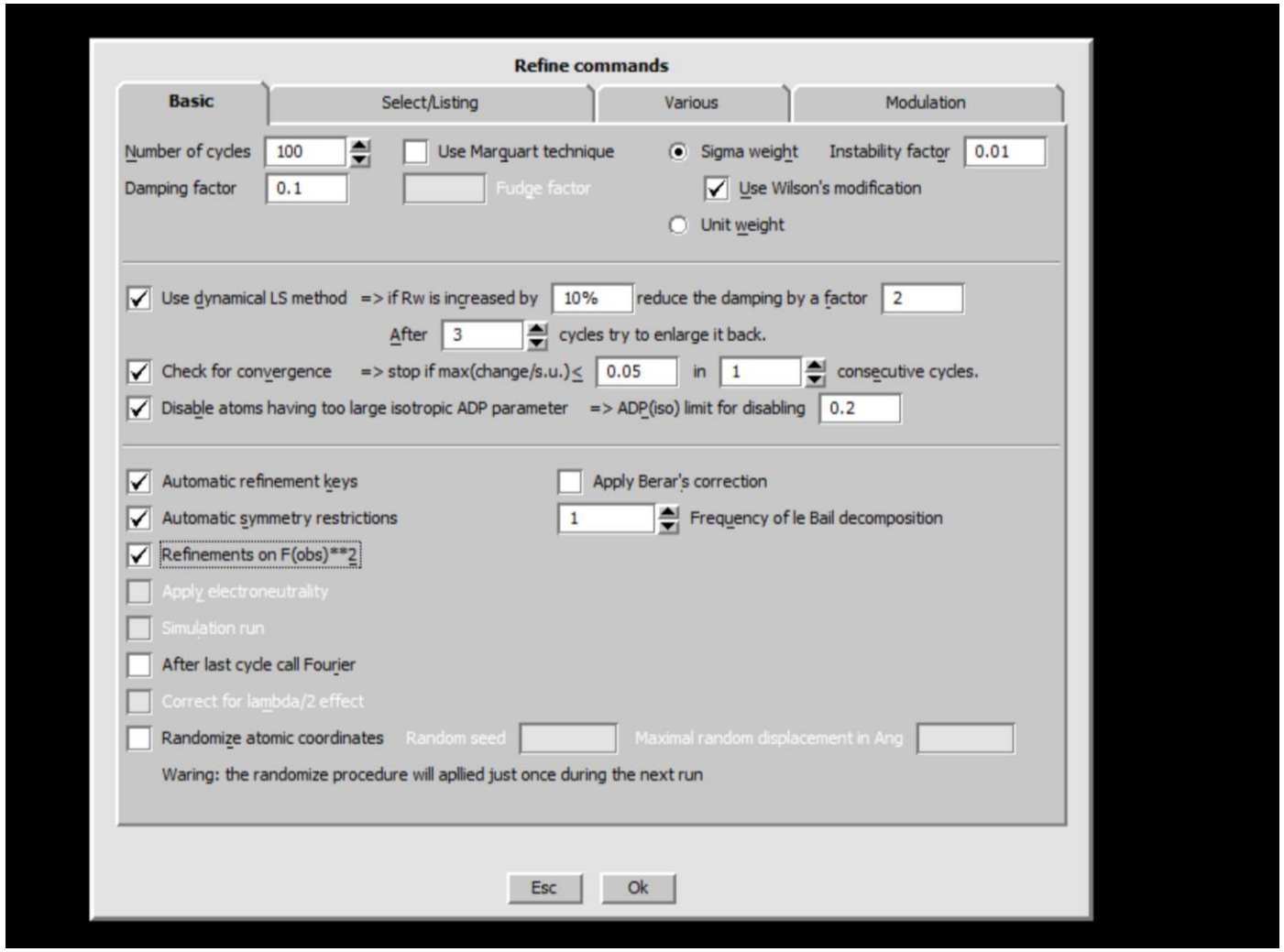
Important!
Refine your peak shape



Important!
Refine your background

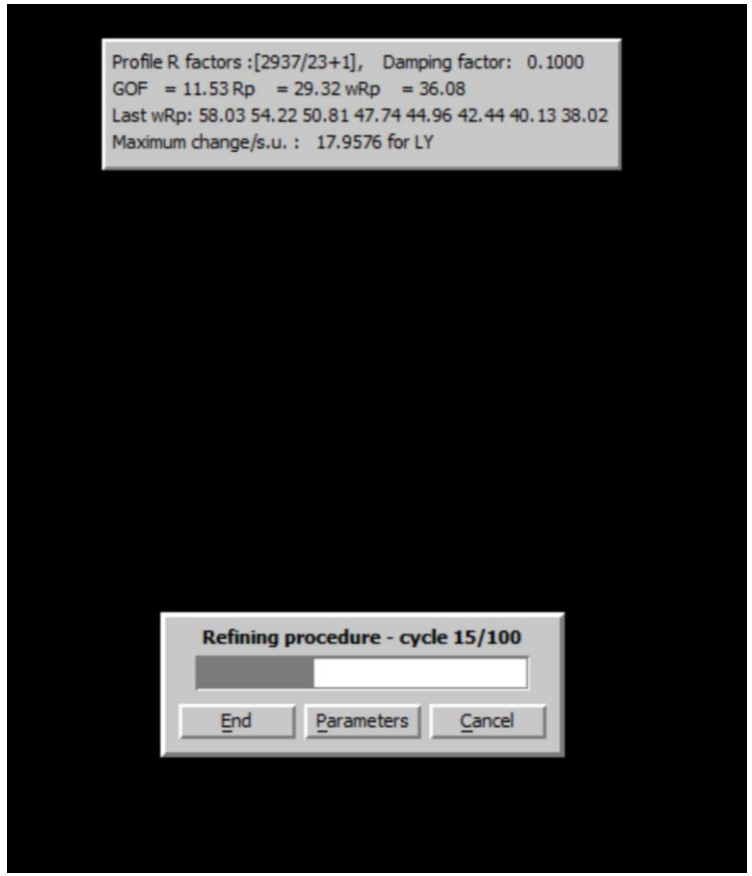


Edit your refinement profile

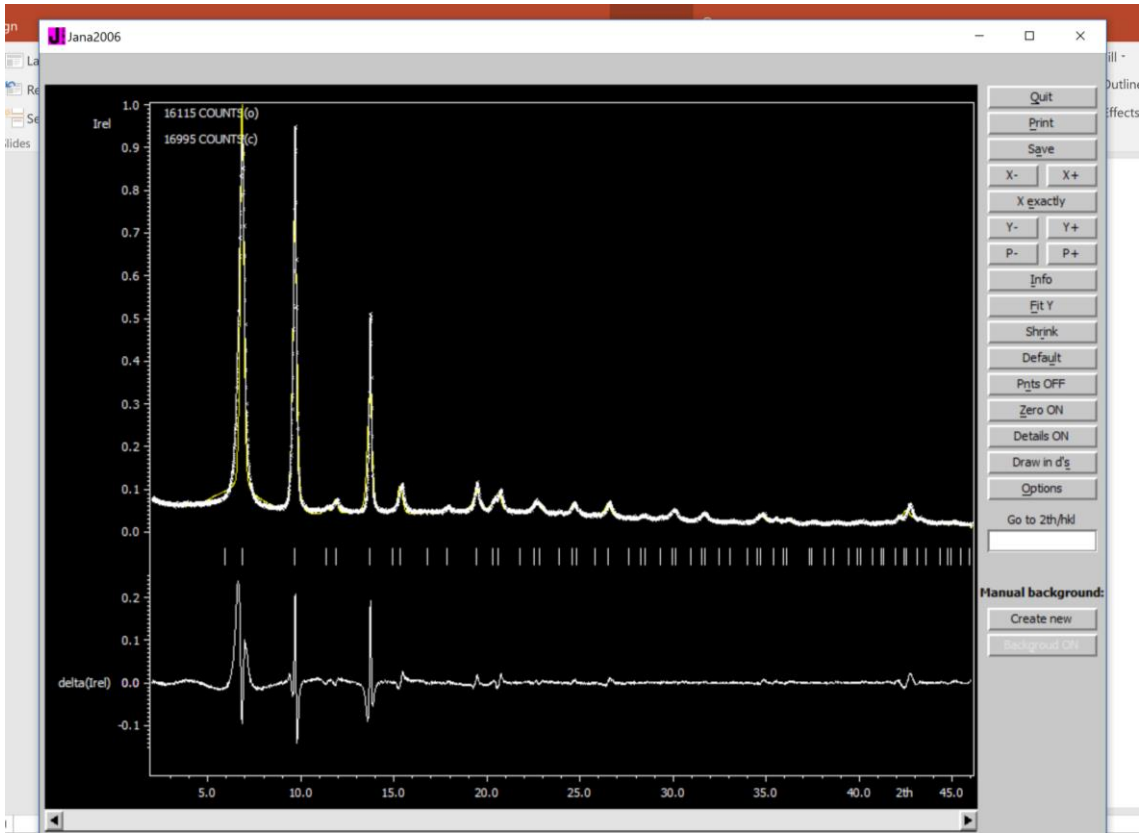


Ready to start refining!

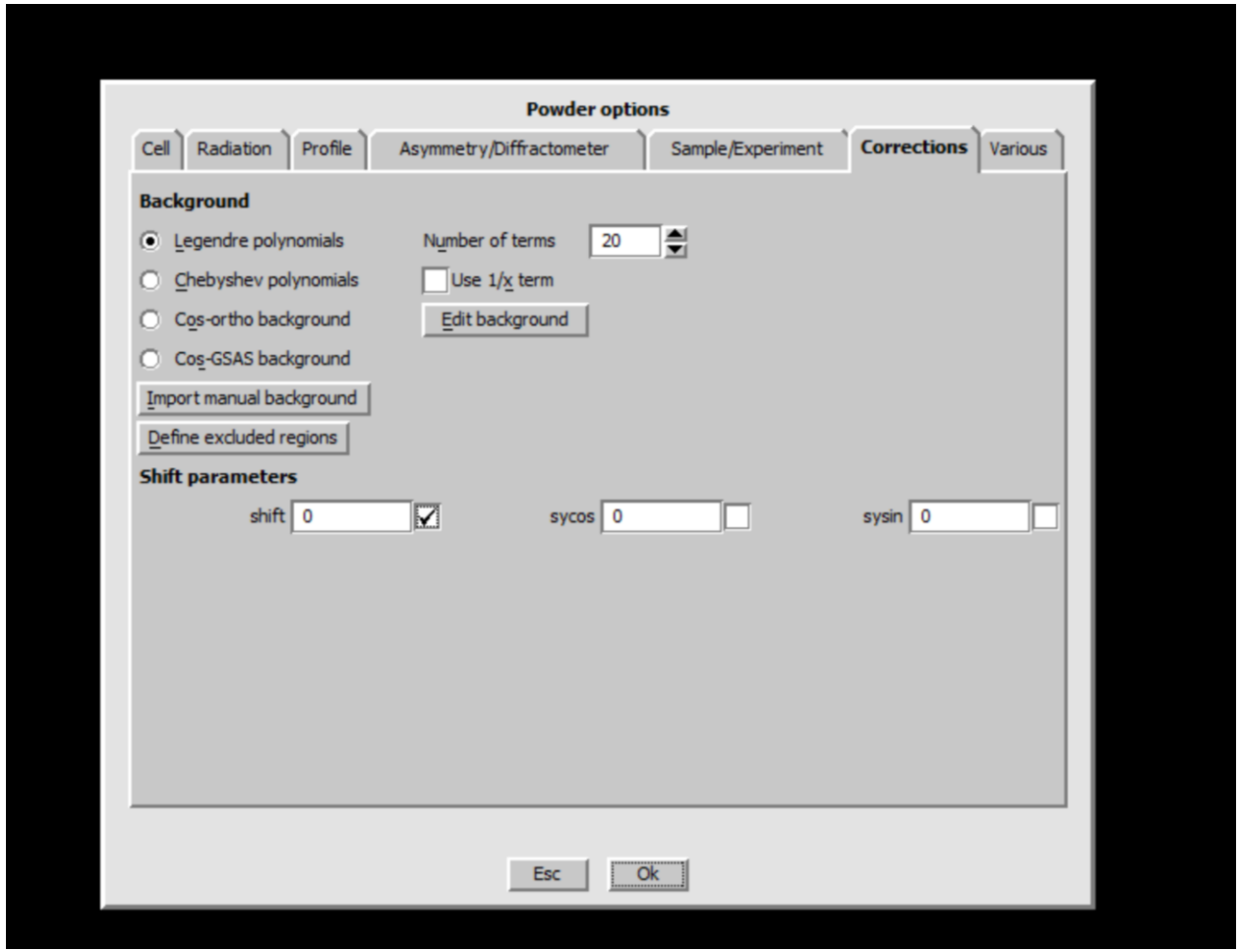
Refinement



At the end of the refinement
check your ptofile



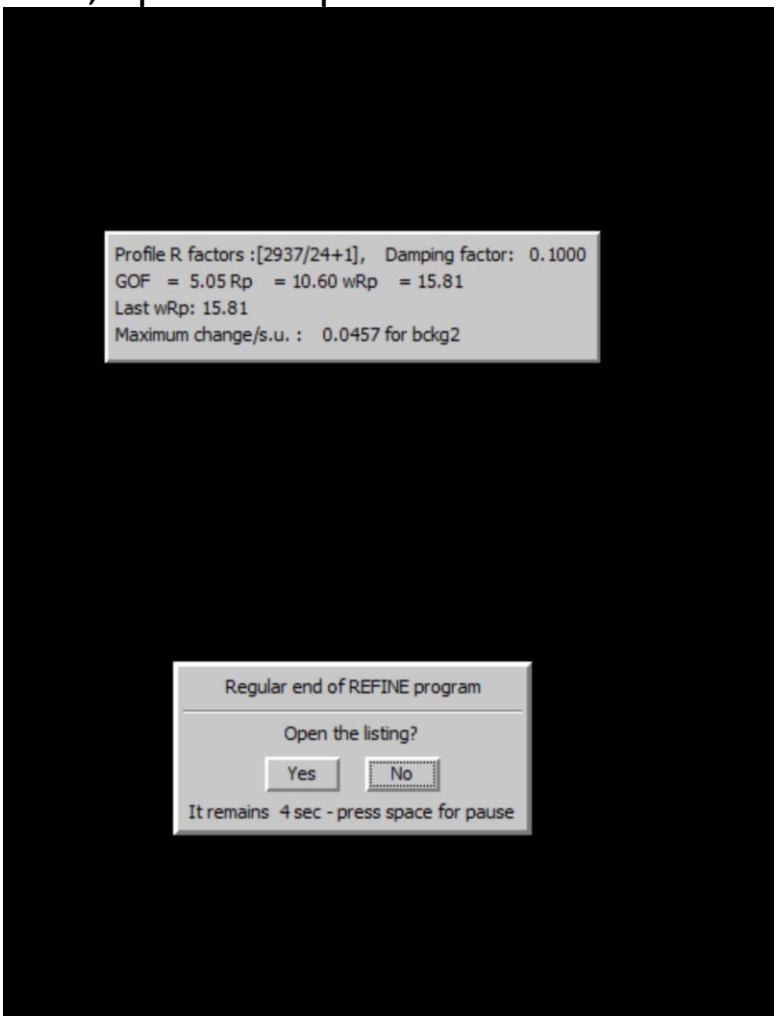
Refinement (modify your profile and repeat)



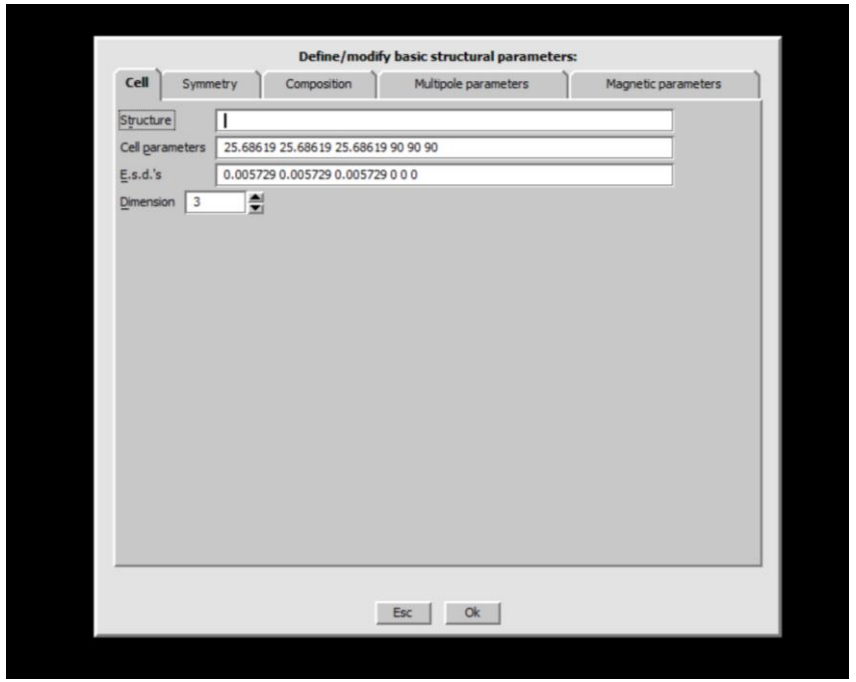
When your powder pattern is close to the experimental one refine the shift (Edit Profile Icon)

Use your data

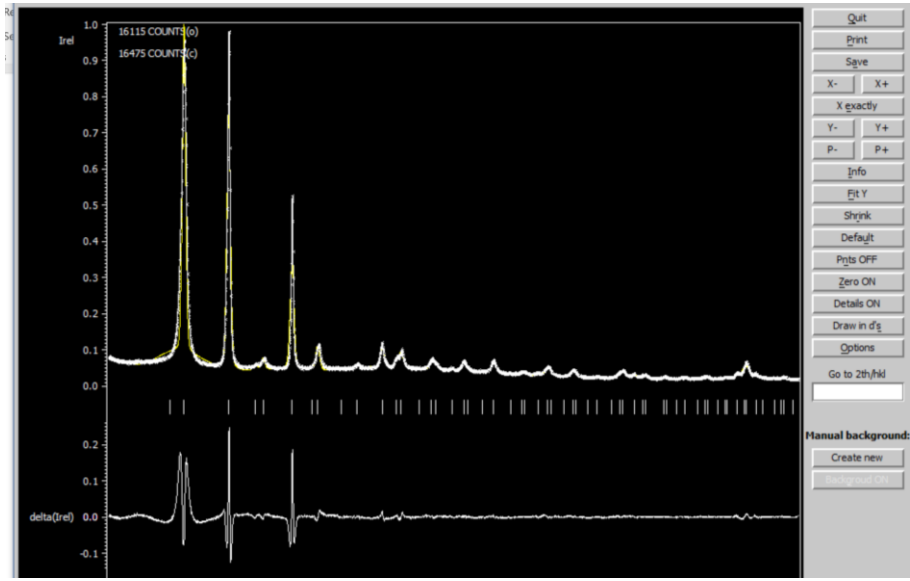
Report your statistics after refinement converges
GOF, Rp and wRp



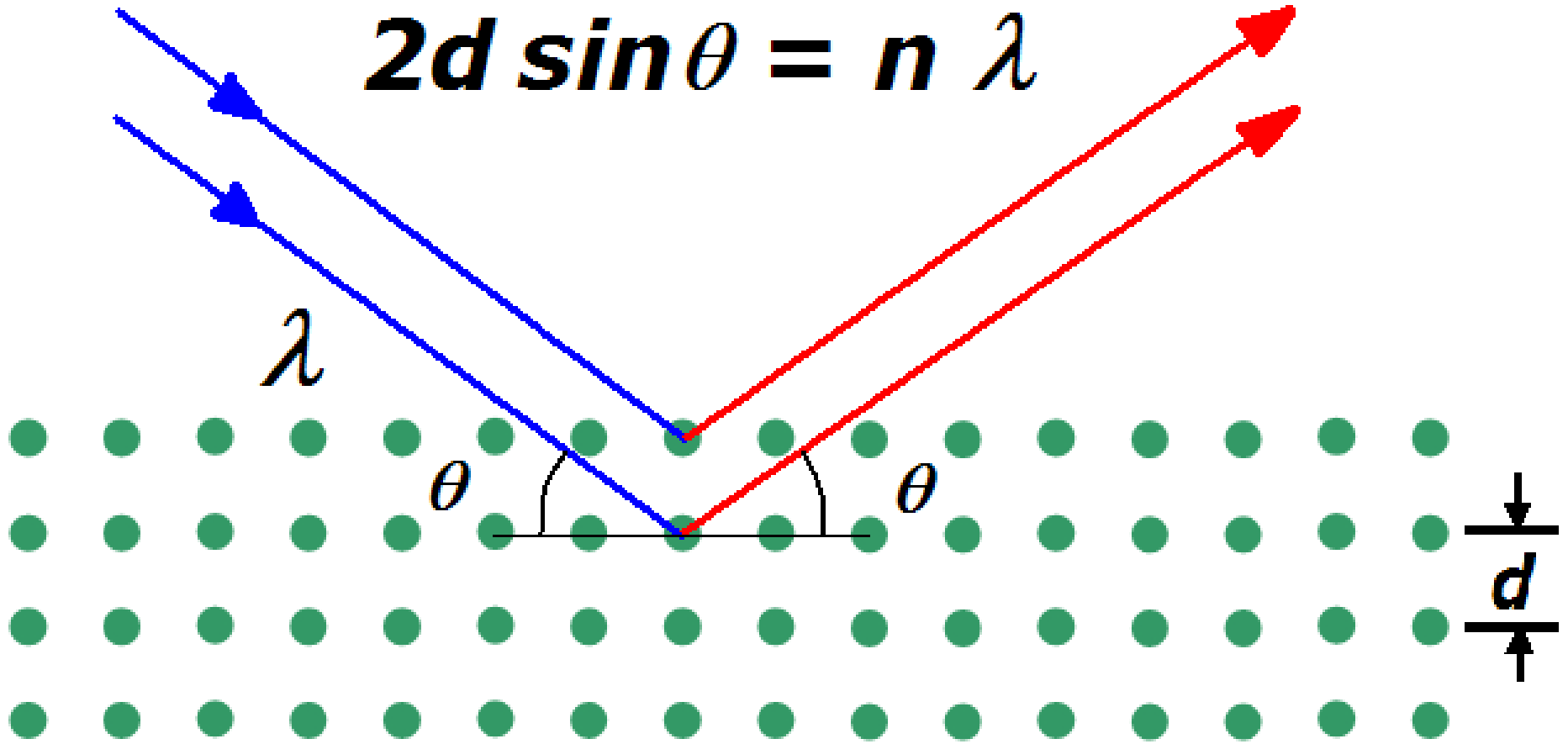
Report your final lattice parameters (Edit M50 Icon)



Plot your data (Profile Viewer Icon)

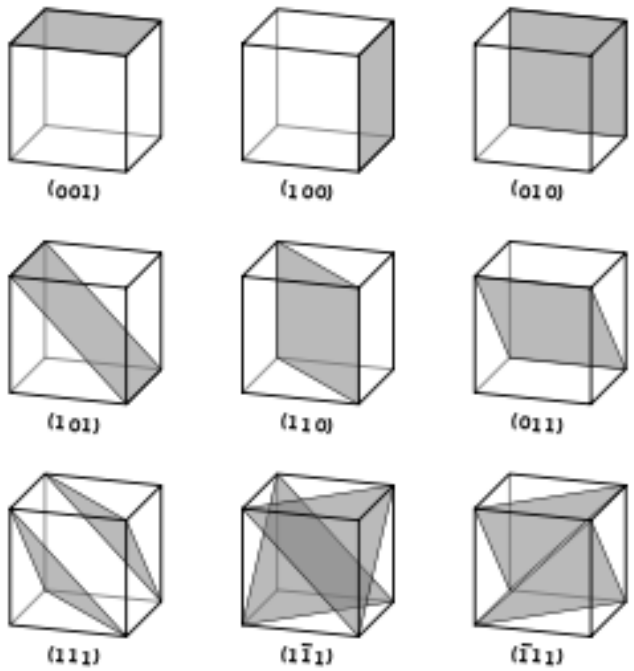


X-ray diffraction: The basic principle

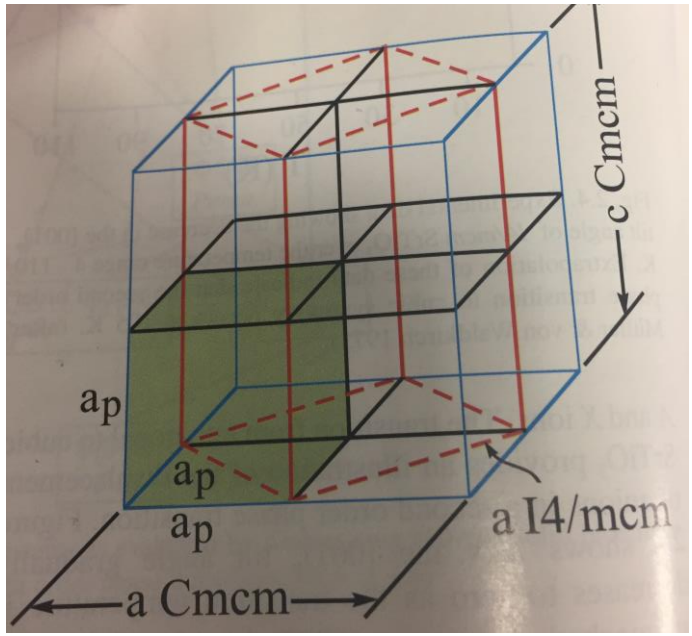


Miller Indices (hkl) of the atom planes

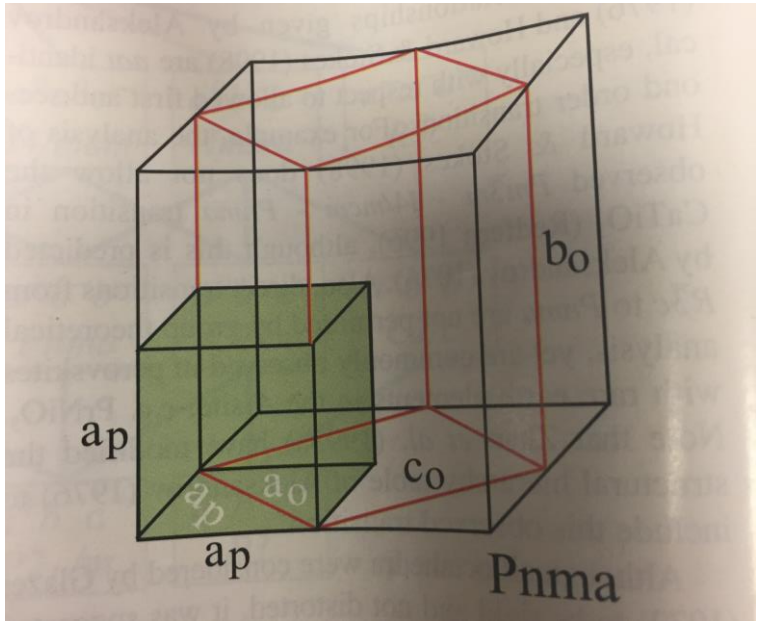
Cubic



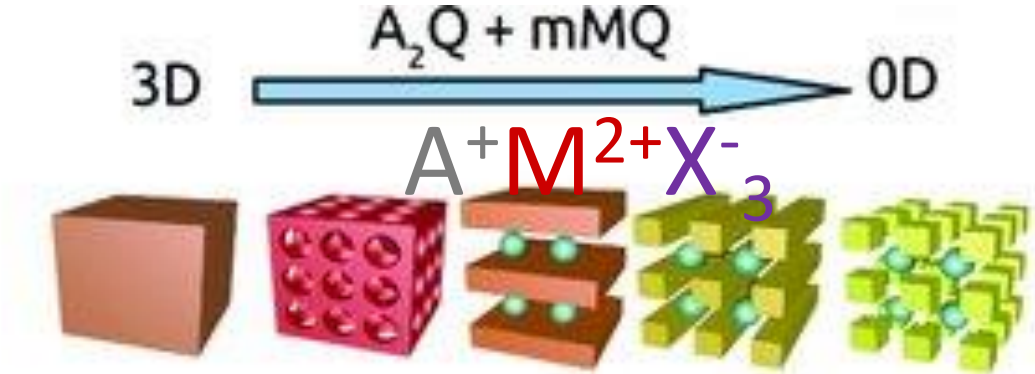
Tetragonal

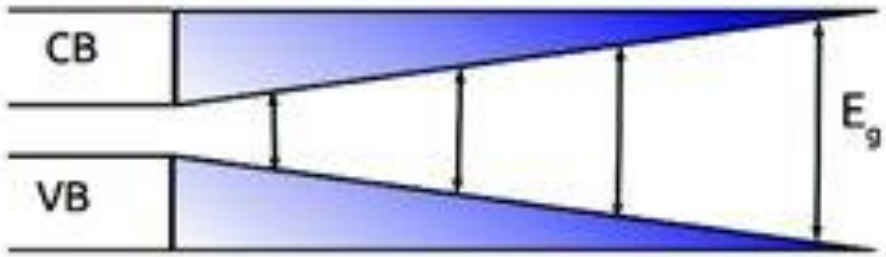


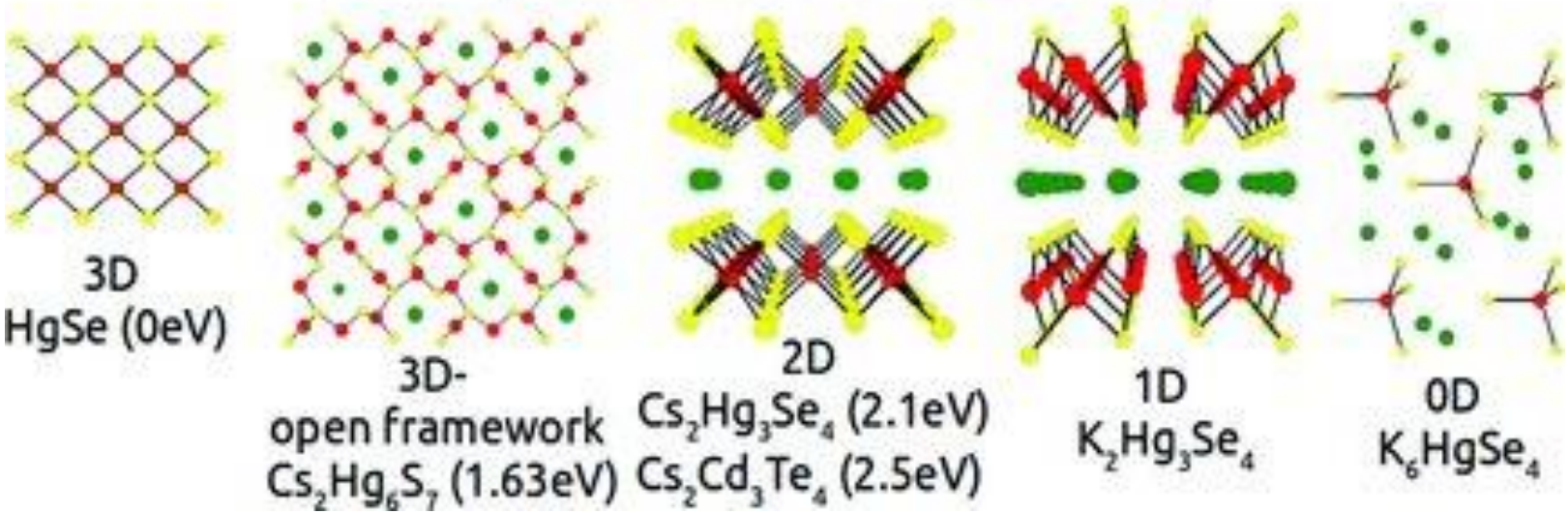
Orthorhombic

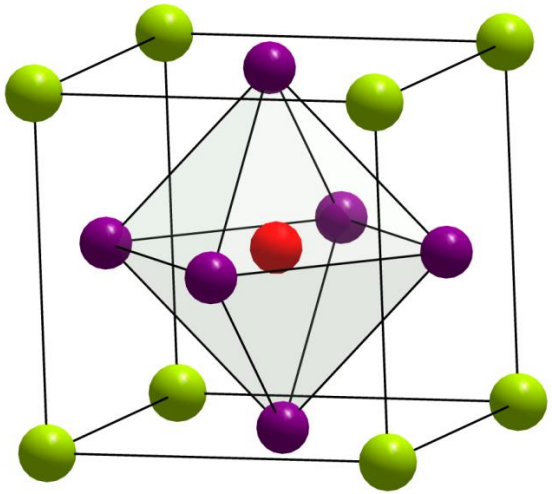


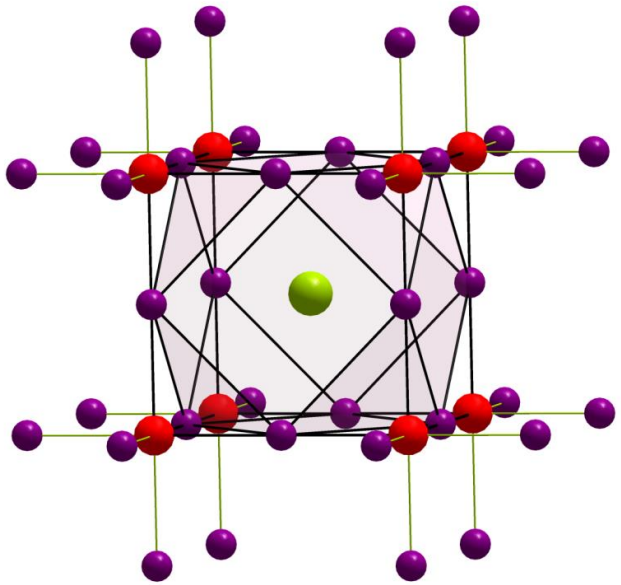
The concept of Dimensional Reduction







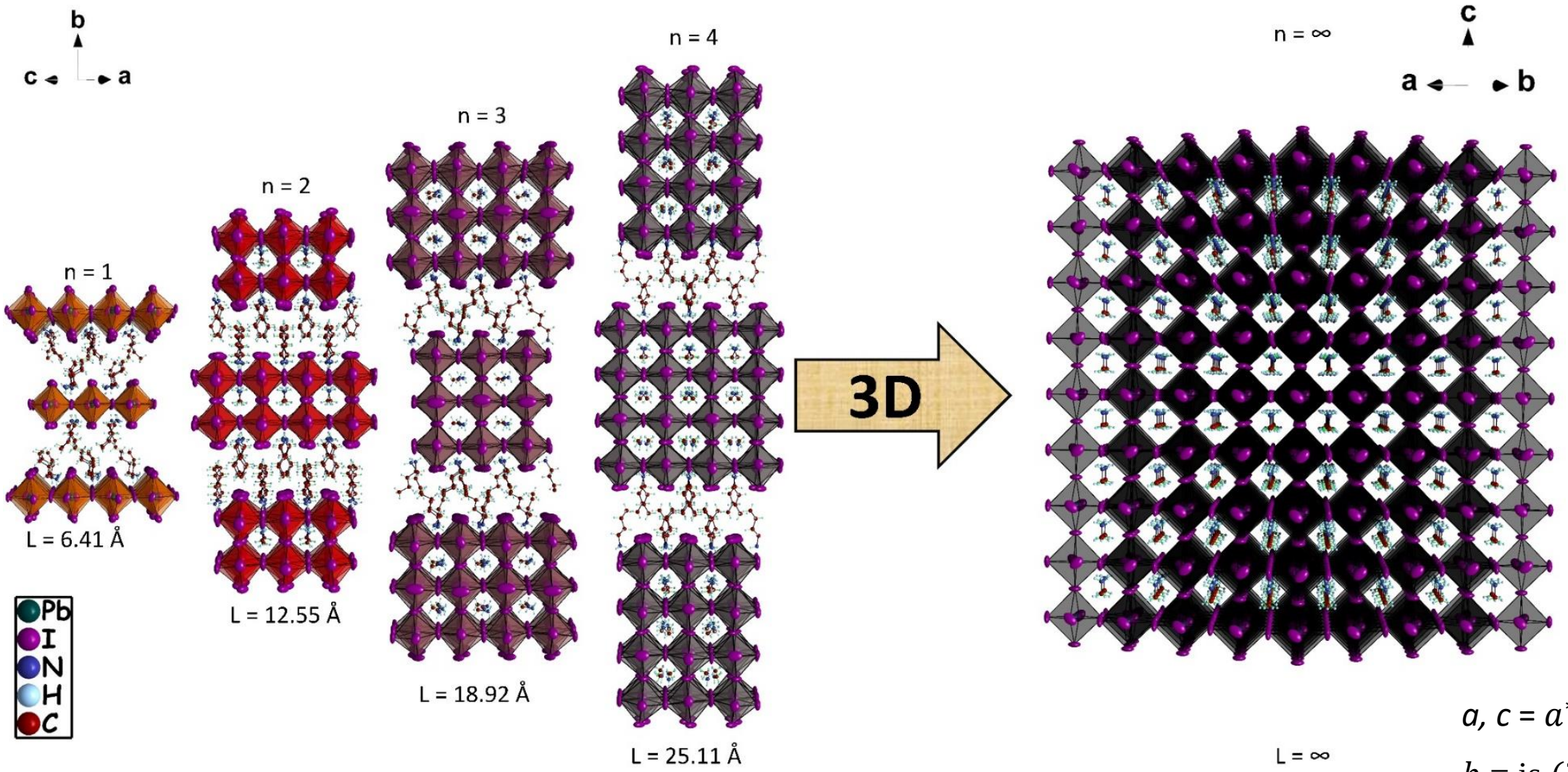




C. C. Stoumpos, M. G. Kanatzidis, *Acc. Chem. Res.* **2015**, *48*, 2791.

Androulakis, J., Peter, S. C., Li, H., Malliakas, C. D., Peters, J. A., Liu, Z., Wessels, B. W., Song, J.-H., Jin, H., Freeman, A. J. Kanatzidis, M. G. (2011), Adv. Mater., 23: 4163–4167

Crystal Structures of $(BA)_2(MA)_{n-1}Pb_nI_{3n+1}$ (n = 1, 2, 3, 4)



$a, c = a^*\sqrt{2}$

b = is $(2a^*n + x)$,

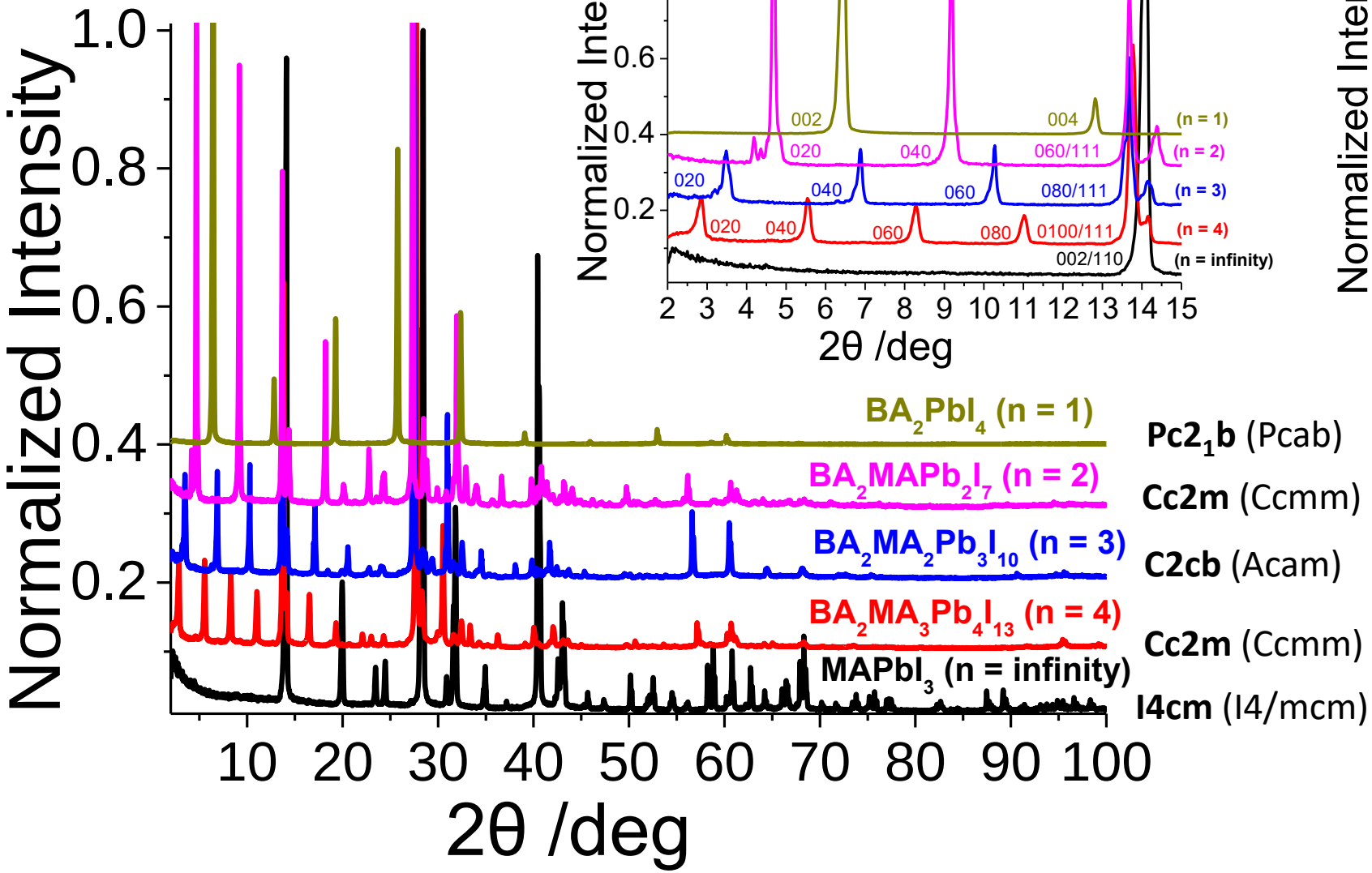
$a^* = 6.3$ Å $(MAPbI_3)$

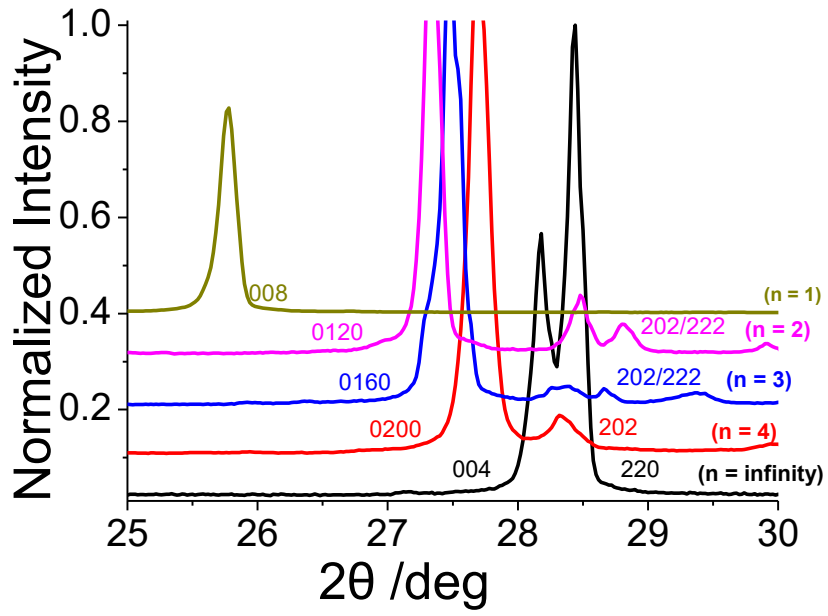
$x \sim 8$ Å $((BA)_2^{2+})$

D. H. Cao, C. C. Stoumpos, O. K. Farha, J. T. Hupp, M. G. Kanatzidis, *J. Am. Chem. Soc.* **2015**, *137*, 7843

C. C. Stoumpos, D. H. Cao, D. J. Clark, J. Young, J. M. Rondinelli, J. I. Jang, J. T. Hupp, M. G. Kanatzidis, *Chem. Mater.* **2016**, *28*, 2852

Powder patterns of 2D materials





Pc2$_1$b (Pcab)

Cc2m (Ccmm)

C2cb (Acam)

Cc2m (Ccmm)

I4cm (I4/mcm)

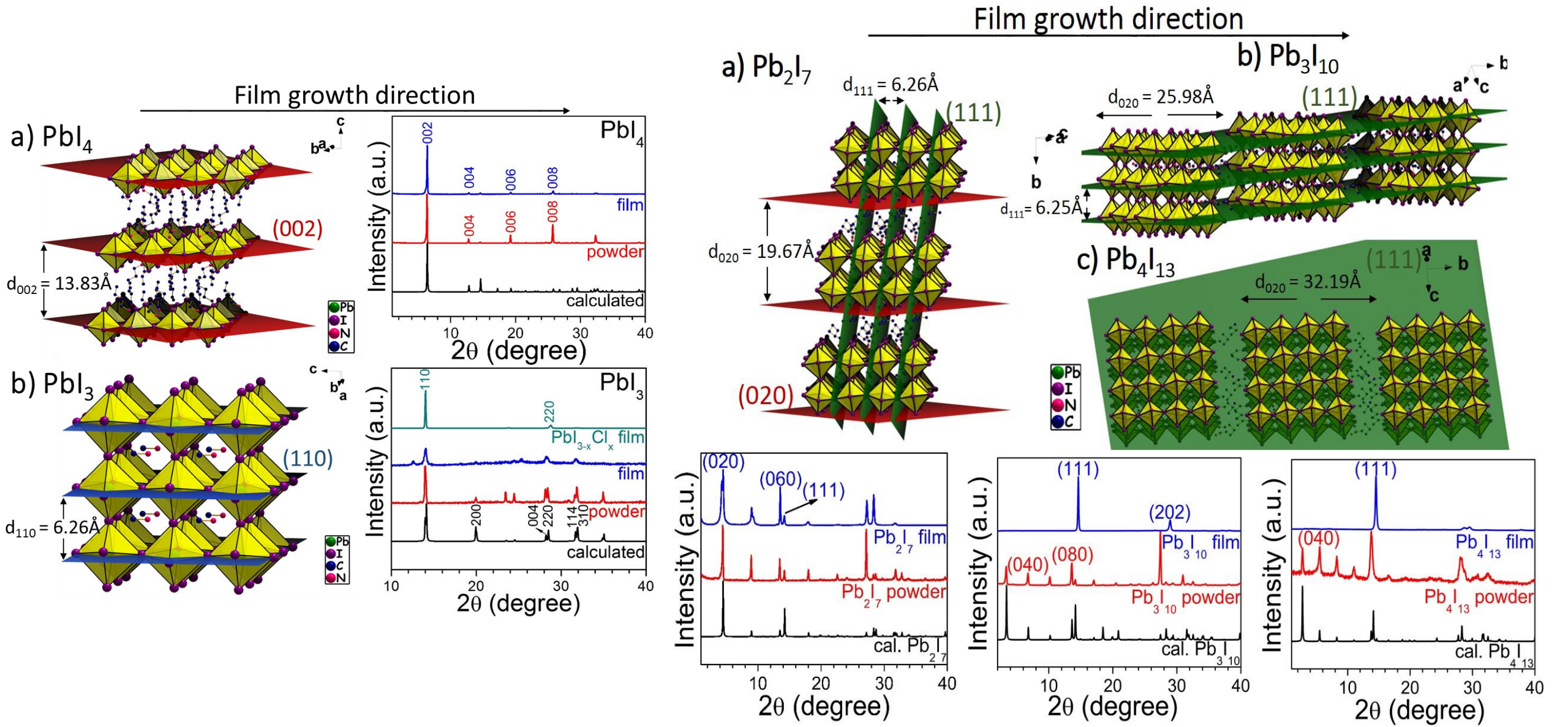
Interplay of space group symmetry:

When **n = even** derives from **Cmcm**

When **n = odd** it derives from **Cmca**

C. C. Stoumpos, D. H. Cao, D. J. Clark, J. Young, J. M. Rondinelli, J. I. Jang, J. T. Hupp, M. G. Kanatzidis, *Chem. Mater.* **2016**, *28,* 2852

Preferred growth orientation Intermediate Members



D. H. Cao, C. C. Stoumpos, O. K. Farha, J. T. Hupp, M. G. Kanatzidis, *J. Am. Chem. Soc.* **2015**, *137*, 7843

C. C. Stoumpos, D. H. Cao, D. J. Clark, J. Young, J. M. Rondinelli, J. I. Jang, J. T. Hupp, M. G. Kanatzidis, *Chem. Mater.* **2016**, *28*, 2852