

Strategy for Rietveld refinement

I) Experiment

- a) Sample
- b) Data Acquisition
 - 1) Choice of Instrument
 - 2) Measuring time
 - 3) Visible problems

II) Refinement

- a) Literature Search
- b) Starting model
- c) "Strategy"
 - 1) Zeroshift, wavelength, background (by hand)
 - 2) Zeroshift, scalefactor, lattice parameters, 1st background parameter
 - 3) Atomic positions, isotropic temperature factor, background parameters
 - 4) Peak shape parameters, asymmetry parameters
 - 5) Individual B factors, atom occupancies
 - 6) Zero displacements
 - 7) Anisotropic B factors
 - 8) Preferred Orientation, microstructural parameters

III) Some Selected Specific Problems

- 1) Peak Intensities: Fourier Difference Map
- 2) Peak Shape: Phase Separation, Microstrain, Size effects

IV) Constraints and Restraints

- 1) Symmetry Constraints
- 2) Constraints due to direct correlation
- 3) Linear Constraints
- 4) Strategic Constraints
- 5) Restraints
- 6) Soft Distance (or Angle) Constraints

} Depends on the
Data quality and the
individual problem

Strategy for Rietveld refinement

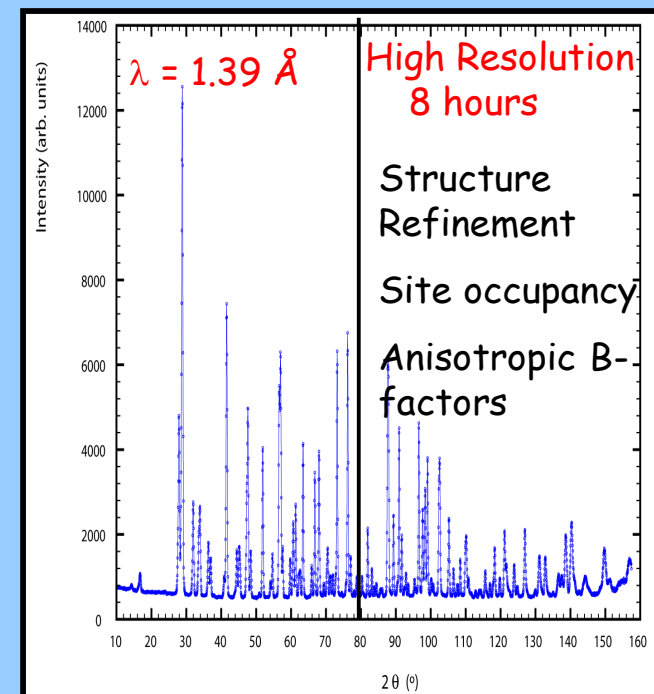
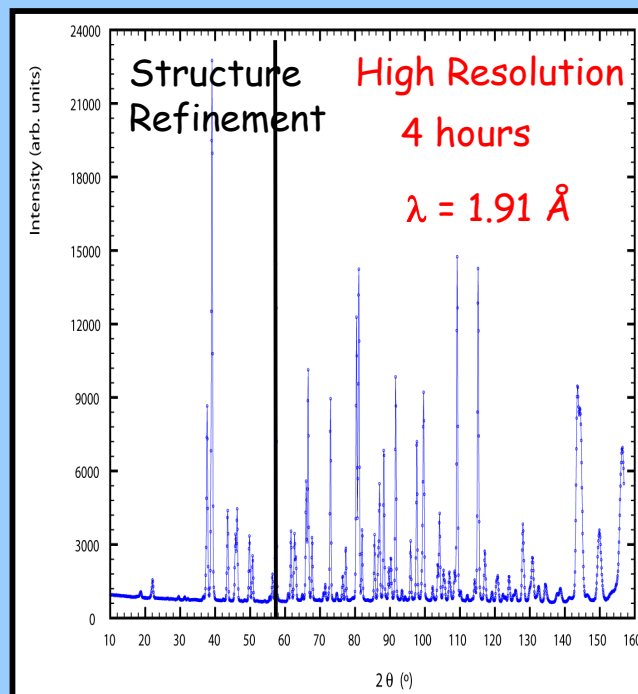
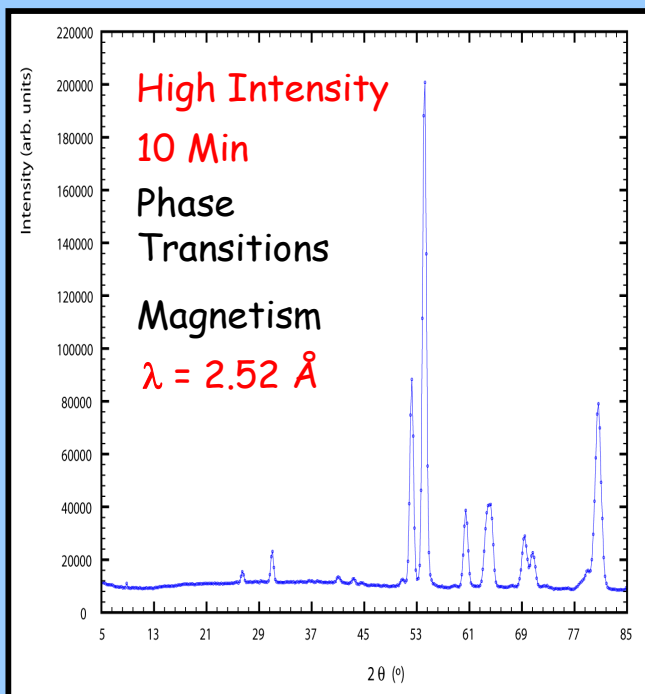
I) Experiment:

a) Sample: **should be impurity free, should be enough** (depending on Instrument and aim), should be well crystallized, avoid the presence of hydrogen (absorbed water)

b) Data acquisition:

1) Choice of instrument: What do I want to find out? Crystallographic structure, phase transition, magnetic structure ... High resolution, high intensity, q-range

Run a standard on the chosen instrument: Determine the zeroshift and the resolution function



Strategy for Rietveld refinement

At an early stage of the measurement : **Always look at the raw data**

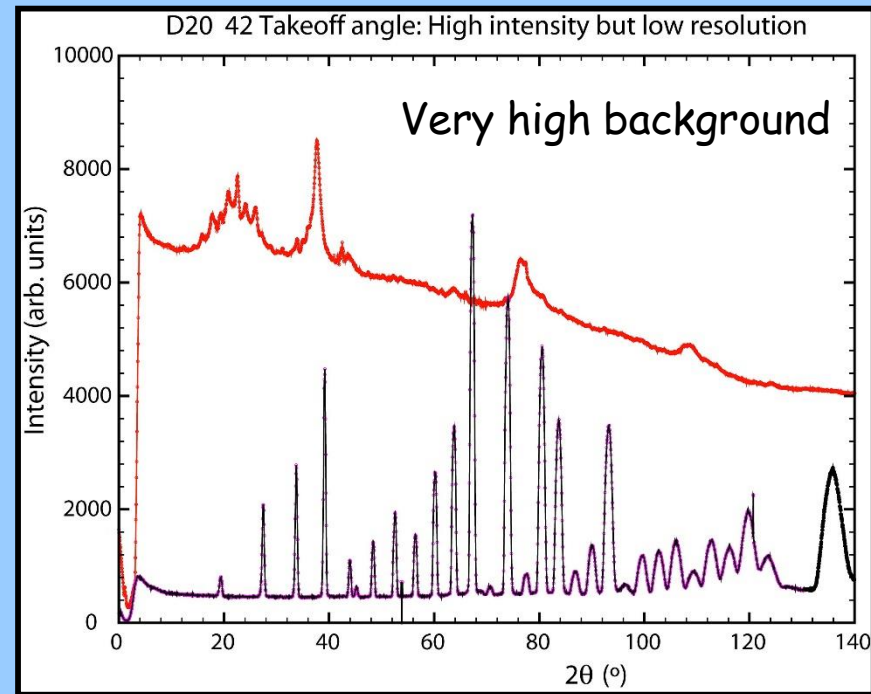
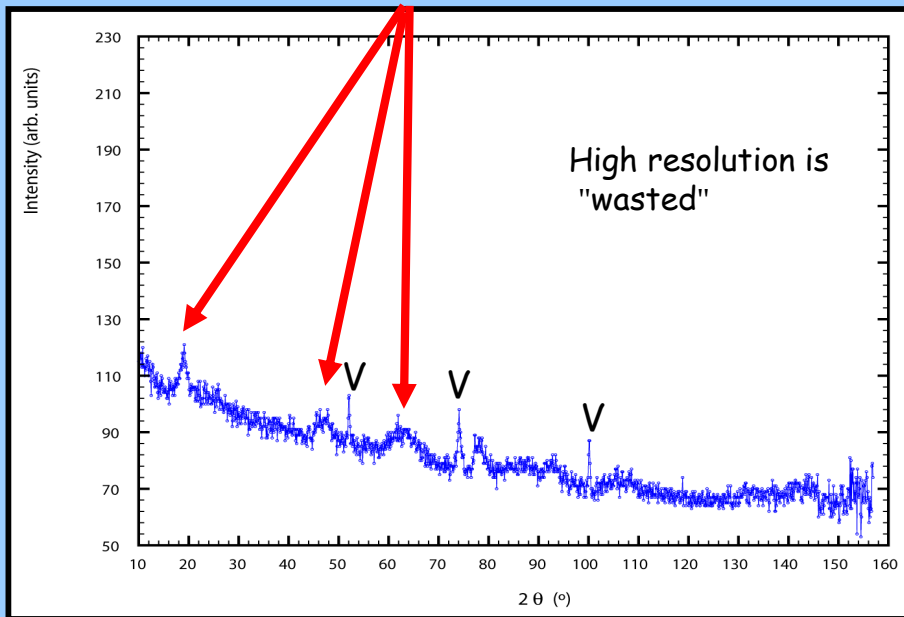
2) Measuring time: Do you see peaks?, Do they have enough intensity?, How do the peaks look like?

3) Visible problems:

Are the peaks only very broad? No good crystallisation, amorphous system? Go to HI machine!

How looks the background? Hydrogen? → Deuteration

"Peaks" from Sample



Strategy for Rietveld refinement

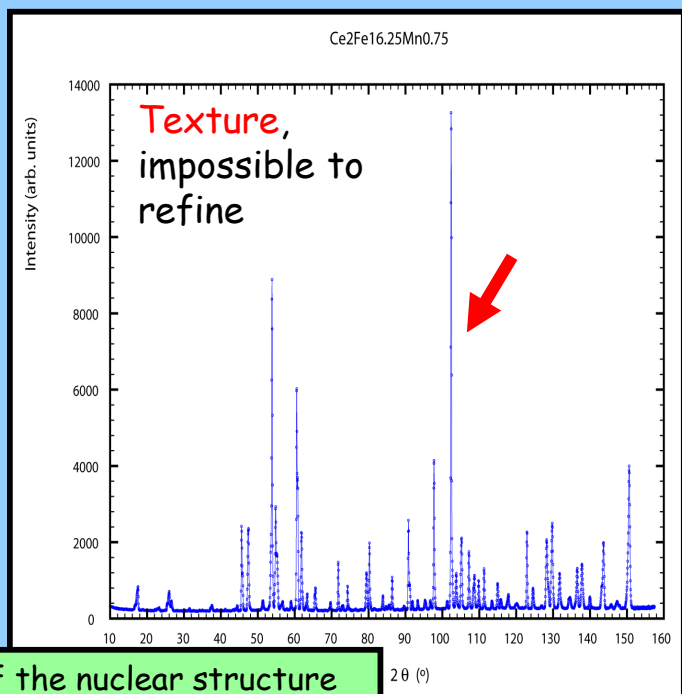
3) Visible problems:

Do the spectra look different between two measurements taking the powder out?

Preferred orientation? (crystallites with layer or needle shape) : Can be corrected for, but try to keep it constant within one measuring cycle (T-dependence).

Are there peaks which are much stronger and sharper than the rest?

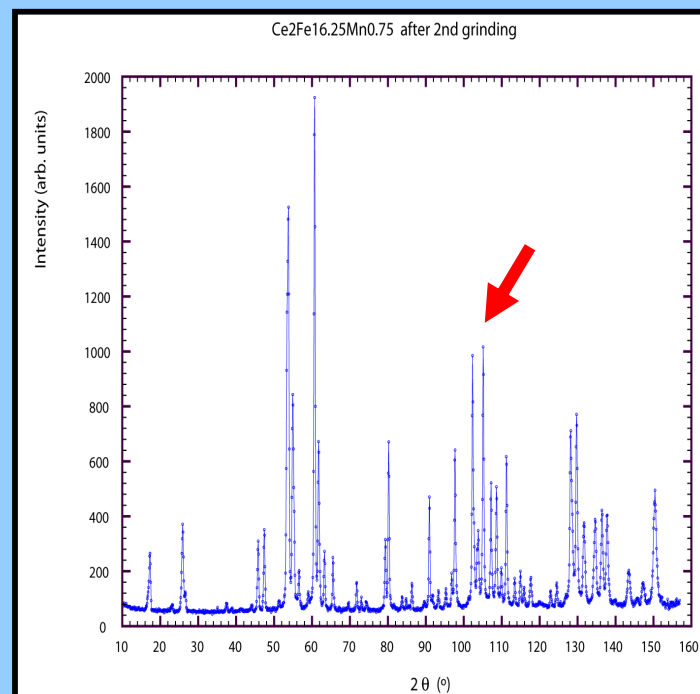
Single crystal!, no powder average = grind further. → **Try to refine as early as possible during the experiment**



If the nuclear structure is not refined correctly you can't get anything for the magnetic structure!

Same sample after grinding twice

Absolute and relative intensities have totally changed!



Strategy is hopeless if the data are not good!

Strategy for Rietveld refinement

II) Refinement

a) Literature Search:

Recuperate all the information you can get from literature about the system studied.

X-ray results of the same compound, Results for similar compounds

b) Starting Model:

In order to start refinement you need a model with lattice constants (**LeBail fit**), spacegroup (**CheckGroup**), and atom positions

Recuperate old pcr file! (one where you know that it works) and introduce your model

Peakshape parameters with starting values from instrument (Standard sample).

c) Strategy:

Run FULLPROFF with zero parameters: Where is the background? Are the peak positions correct?

If not: Are the shifts between calculated and observed peak positions similar: zeroshift wrong

Are the shifts q-dependant: lattice constants wrong or wavelength wrong

In order to refine the lattice constants the cal/obs peak positions must at least partially overlap,

Start with small 2 Theta range at great d-spacings first.

Background can be put at suited starting value by hand.

Strategy for Rietveld refinement

Refine the zeroshift, the scalefactor and the lattice constants.

Always keep a "reserve" pcr file in case the program diverges.

(Put the parameter "pcr" = 2, this creates a *.new file conserving the *.pcr file)

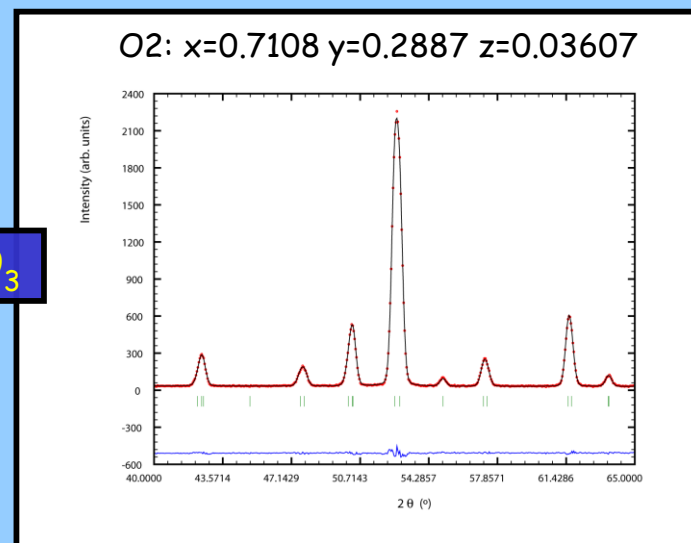
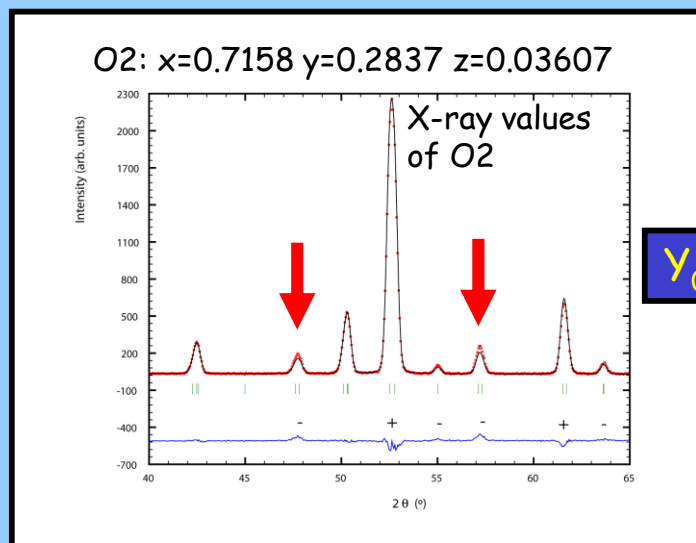
As long as the program did not "lock in", no sense to continue!

Always follow the progress of the refinement by looking at the resulting fit!

Refine the atomic positions (which are free to move), an isotropic temperature factor and the background

Wrong atom position: Difference curve shows "ups" and "downs",

very sensitive to Oxygen position → be careful with from x-ray data determined structures containing Oxygen

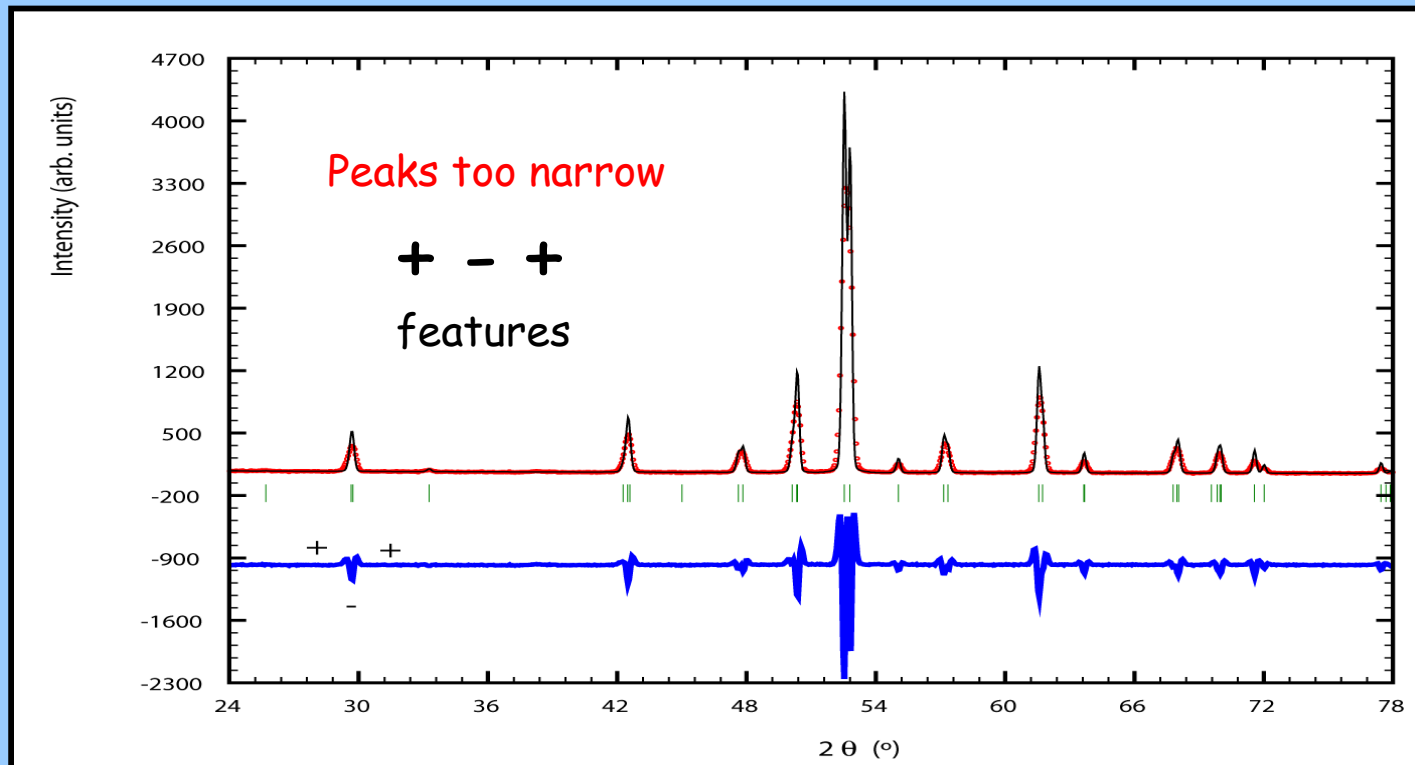


Strategy for Rietveld refinement

Refine Peakshape parameters and asymmetry parameters

Wrong lineshape parameters: Calculated peakshape too narrow

Always better to start with a too narrow peakshape! A too broad peakshape hides the real problems!

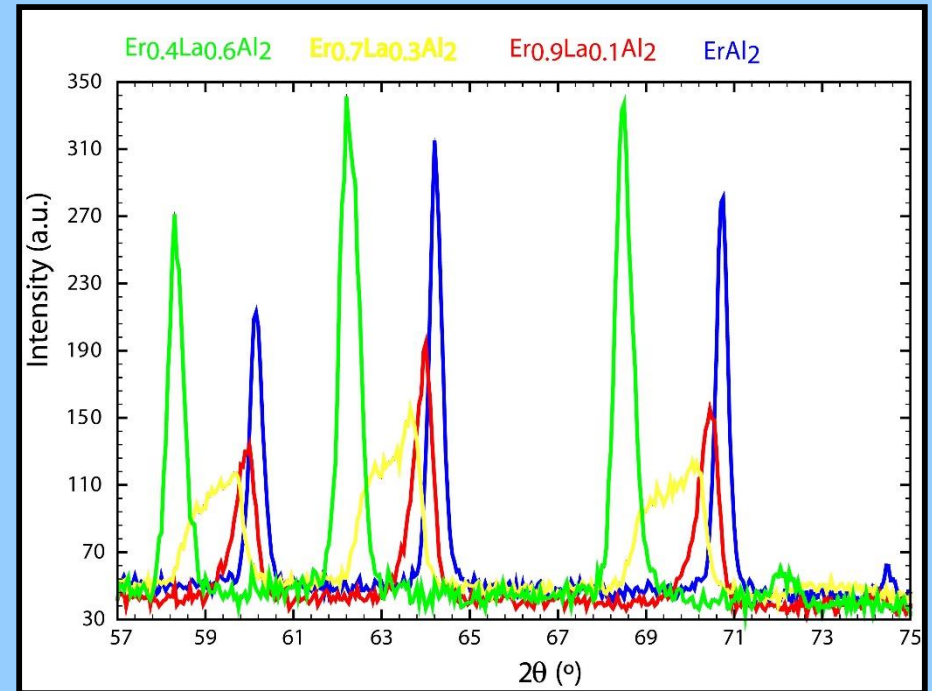
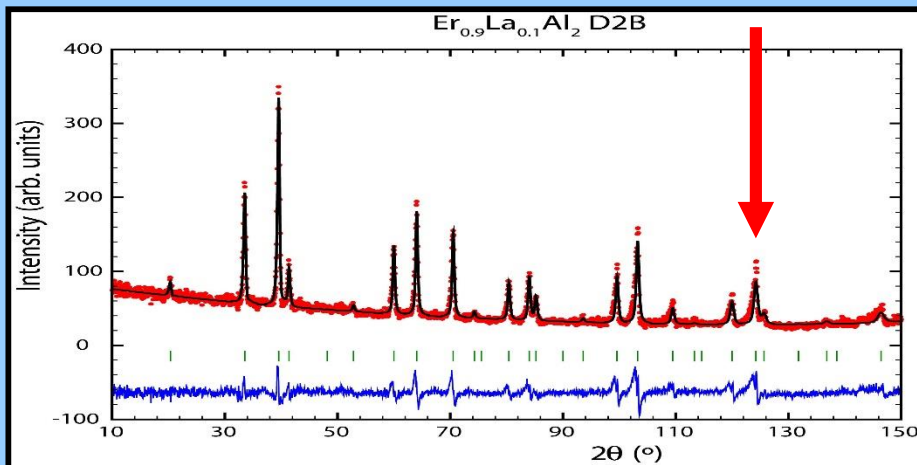
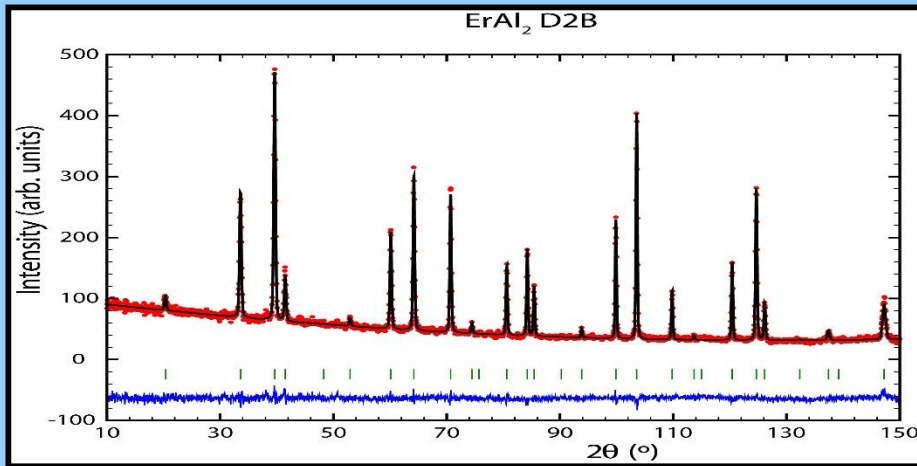


Strategy for Rietveld refinement

Wrong lineshape parameters: Calculated peakshape too large

R-factor = 4! Look at the plot!

The broad lineshape of the calculated pattern accounts partially for the wrong model!



Inhomogeneous system: $\text{Er}_{1-x}\text{La}_x\text{Al}_2$

No symmetry reduction but a distribution of cubic unit cell parameters

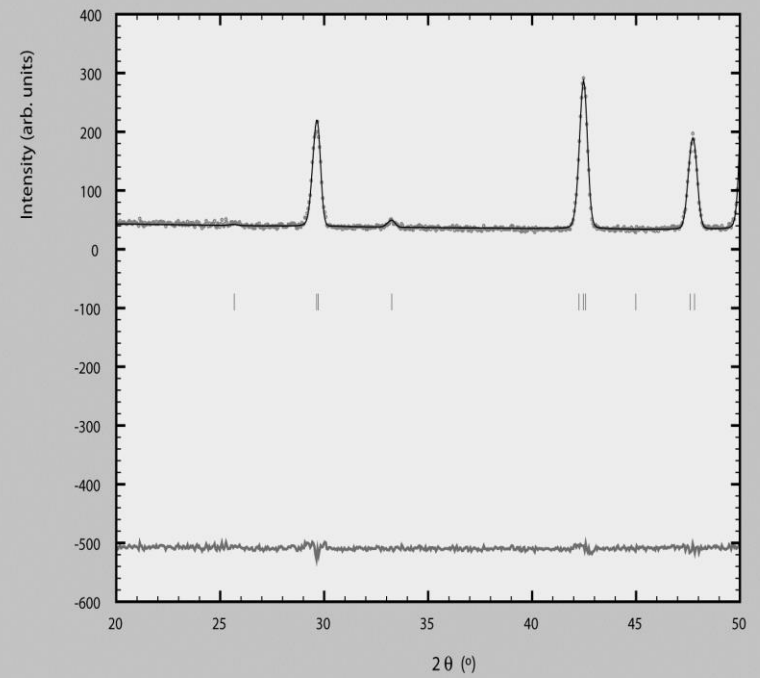
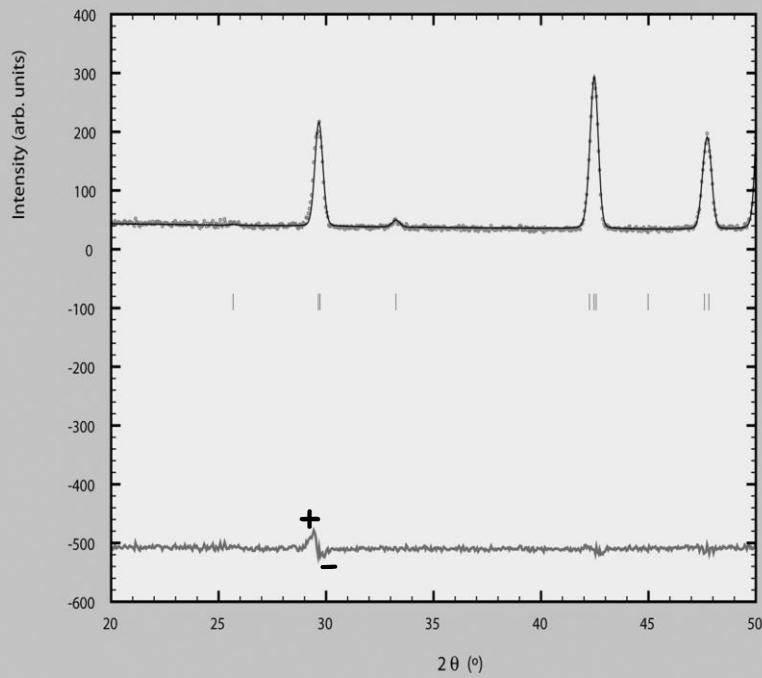
as system is not behaving as a solid solution

Strategy for Rietveld refinement

Influence of Asymmetry parameters

Mainly important at low angles

Typical $+$ $-$ pattern in the difference curve



Strategy for Rietveld refinement

Practical Example: $\text{YFe}_3(\text{BO}_3)_4$, neutron data at 295 K ($1.91\text{\AA}$) and 520 K ($1.39\text{\AA}$)

Already known: $\text{TbFe}_3(\text{BO}_3)_4$, recuperate the pcr file

[..\..\FullProf_Suite\winplotr.exe](#)

II Refinement

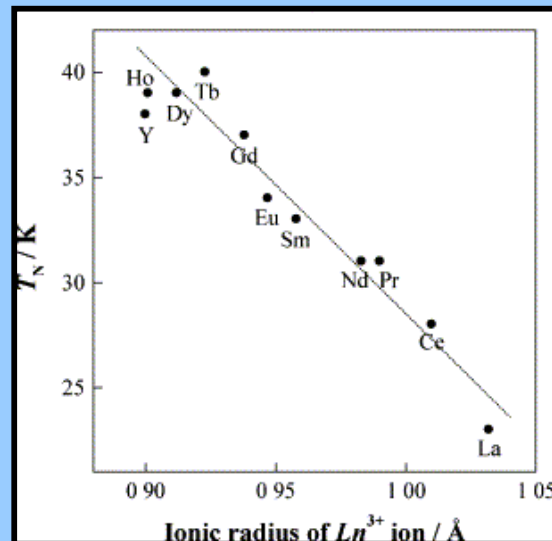
a) Literature search:

1) J.A. Campa et al., Chem. Mat. 1997, 237:
Wyckoff positions are given

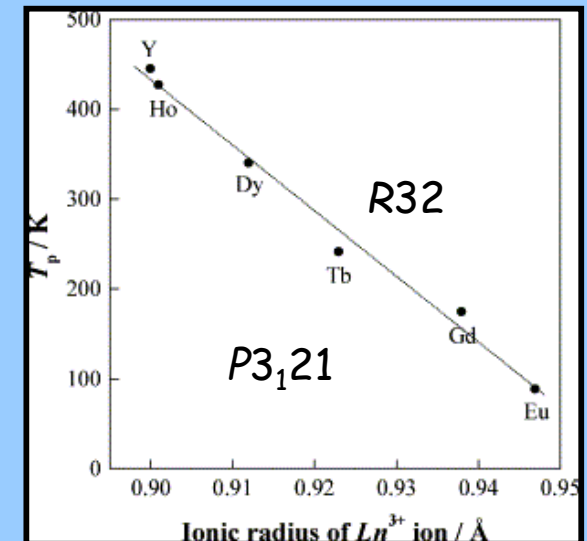
$\text{RFe}_3(\text{BO}_3)_4$ series: Trigonal Huntite type structure, $R32$,

2) Y. Hinatsu et al. J. Sol. St. Chem. **172** (2003) 438:

Magnetic transition
temperature:
Y-compound non
magnetic at RT



Crystallographic
phase transition:
Y-compound at
RT in same phase
as Tb-compound
below 240 K



3) S.A. Klimin et al., Acta Cryst. **B61** (2005) 481: Low temperature structure of $\text{GdFe}_3(\text{BO}_3)_4$ is $P3_121$

Strategy for Rietveld refinement

b) Starting Model:

In order to start refinement you need a model with lattice constants (**LeBail fit**), spacegroup (**CheckGroup**), and atom positions

Recuperate old pcr file! (one where you know that it works) and introduce your model:

Already known: $\text{TbFe}_3(\text{BO}_3)_4$, recuperate the pcr file

Fp

Peakshape parameters with starting values from instrument (Standard sample).

c) "Strategy "

- 1) Zeroshift, wavelength, background (by hand)
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Strategy for Rietveld refinement

III) Some Selected Specific Problems:

1) Wrong peak intensities, but all atom positions refined → Ferromagnetic? (Fe above RT!)

=> Phase No. 1 NUCLEAR

P 6₃/mcm

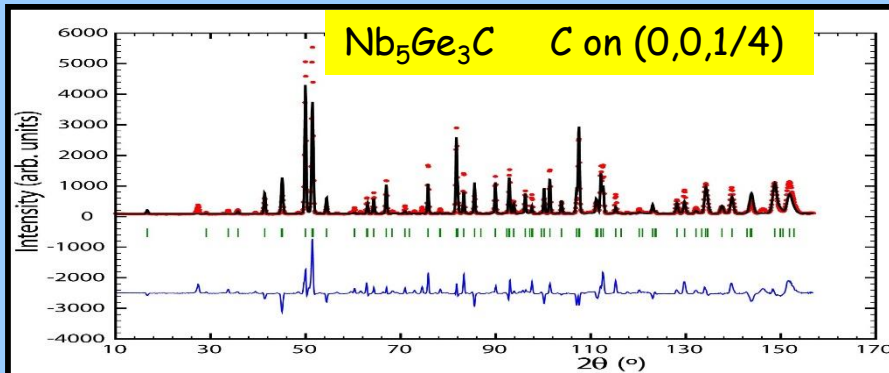
=> No. of reflections for pattern#: 1: 70

==> ATOM PARAMETERS:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.
Nb1	0.33333 (0)		0.66667(0)		0.00000(0)		-0.164(103)		0.167 (0)	
Nb2	0.23783 (69)		0.00000(0)		0.25000(0)		-0.164(103)		0.250 (0)	
Ge1	0.59901 (74)		0.00000(0)		0.25000(0)		0.303(126)		0.250 (0)	
C1	0.00000 (0)		0.00000(0)		0.25000(0)		0.544(0)		0.006 (2)	should be about 0.075

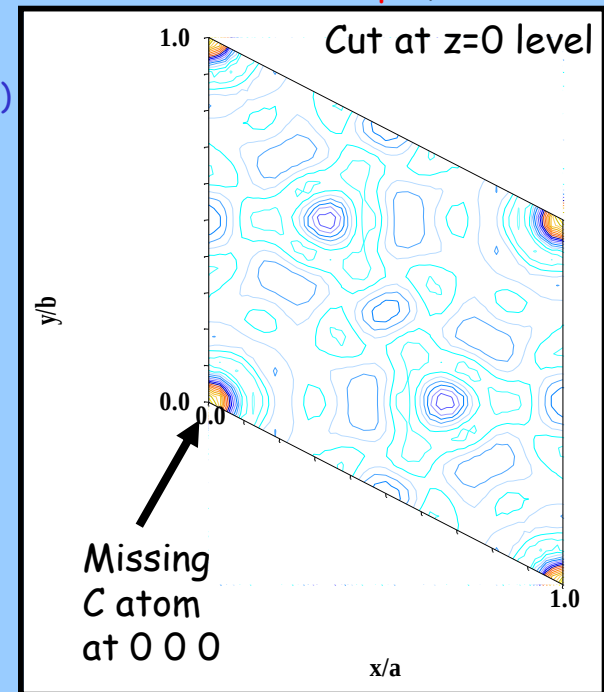
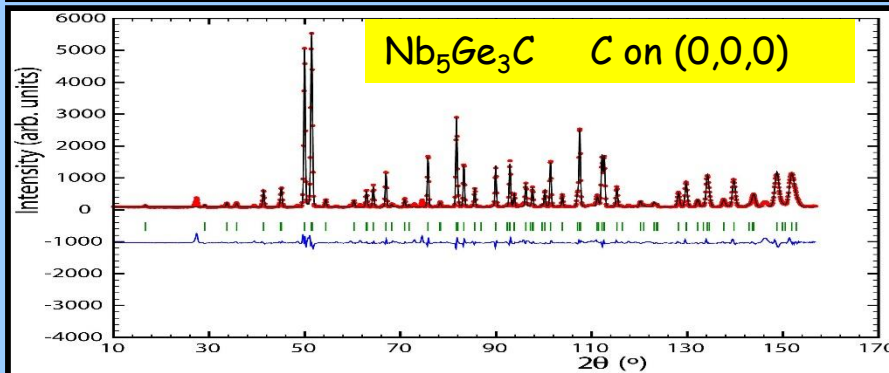
Don't refine now
anisotropic B-
factors!! Will always
give better R-values ...

→ Fourier Difference Map (FOU=4 in pcr file)



Pcr file with C on (0 0 ¼)

Fp



Strategy for Rietveld refinement

III) Some Selected Specific Problems:

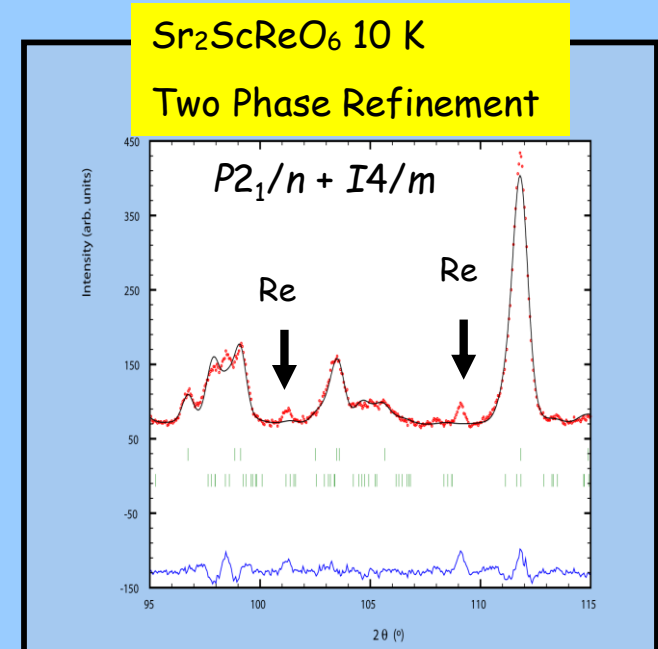
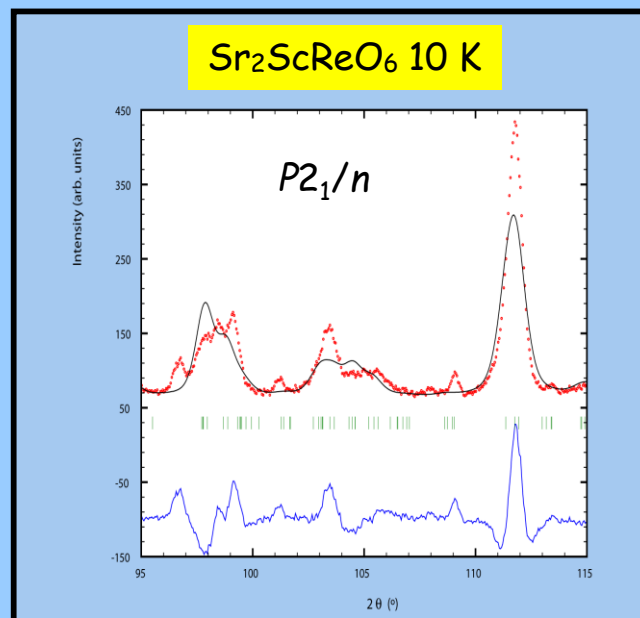
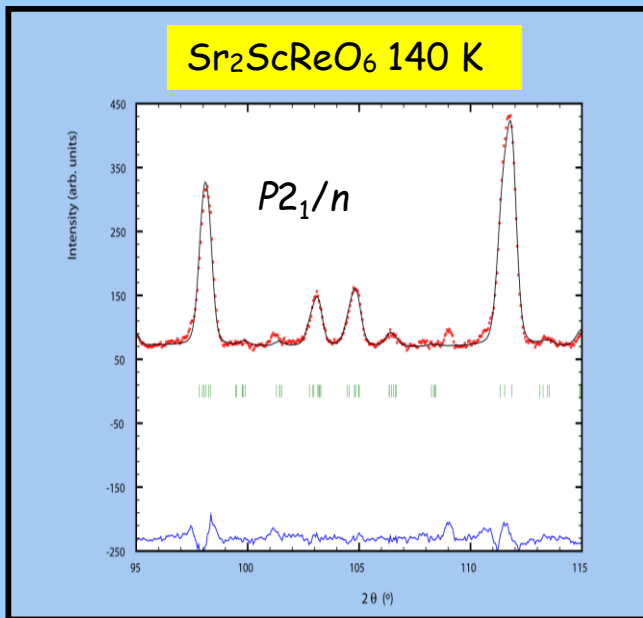
2) Peak Shape:

Peak Broadening, Change the model or use more parameters?

Symmetry reduction (classic), **phase separation**, microstrain, size effects

Phase separation: no chance of indexing, look at the evolution with temperature, peak broadening even for peaks with multiplicity 2!

Fp



Sr₂ScReO₆: Reentrant phase transition: High temperature *I*4/*m* → *P*₂₁/*n* → Low temperature *P*₂₁/*n* + *I*4/*m*

Strategy for Rietveld refinement

III) Some Selected Specific Problems:

2) Peak Shape:

Peak Broadening, Change the model or use more parameters?

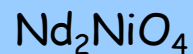
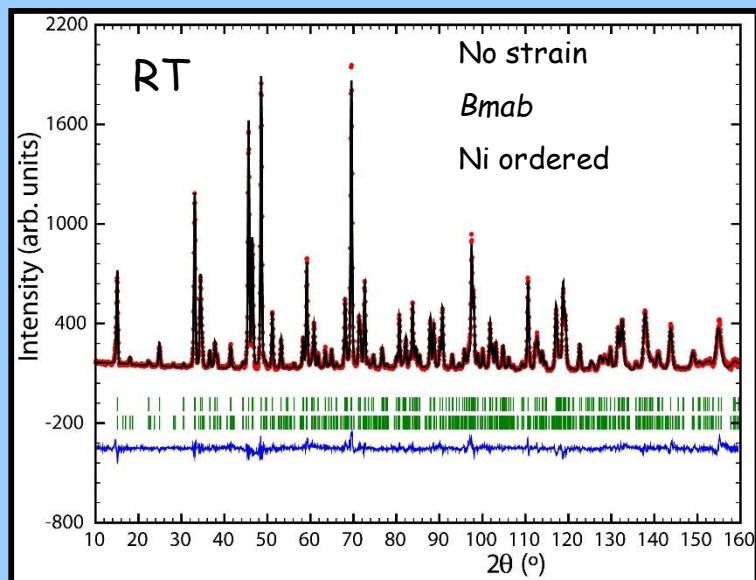
Symmetry reduction (classic), phase separation, **microstrain, size effects**

Microstrain, size effects, how are they visible?

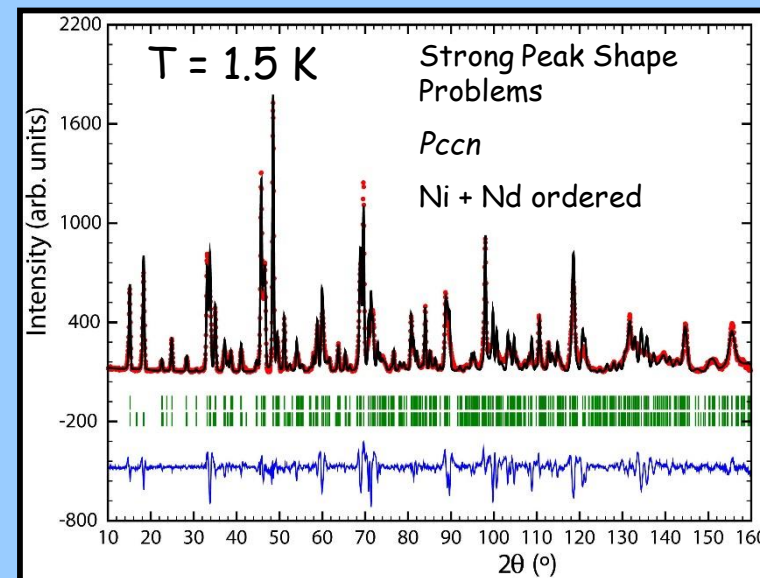
Peak broadening already at low 2θ : **size effect**, at high 2θ : **strain**,

Refinement: Use the instrument resolution "irf" file (Res = 1 in pcr file) and

"U" and "X" for **isotropic strain** and "GauSiz" and "Y" for **isotropic size**



Structural transition
from *Bmab* at high
temperature to *Pccn*
at low temperature



Strategy for Rietveld refinement

III) Some Selected Specific Problems:

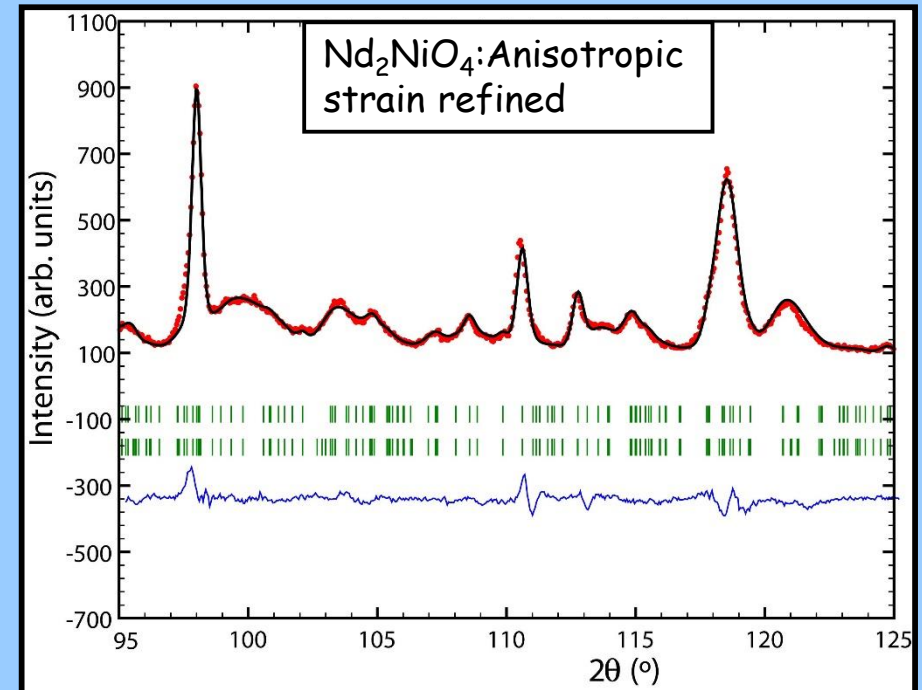
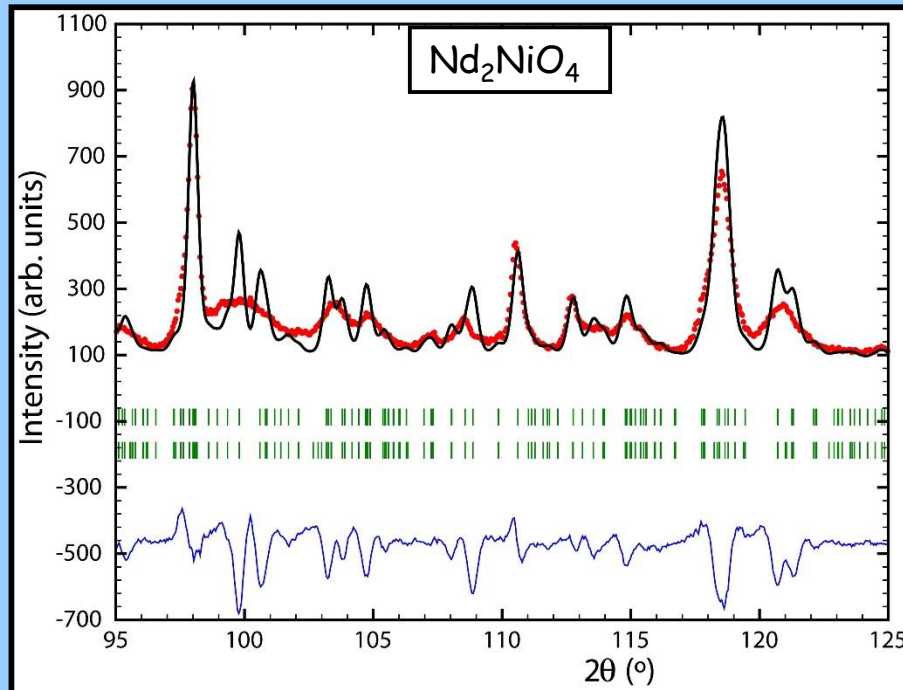
2) Peak Shape:

Nd_2NiO_4 :

Problem linked to **anisotropic Microstrain**:

Some peaks are calculated to broad, others to narrow and some nearly perfectly well!

In order to refine **anisotropic microstrains** (or anisotropic size effects) one has to choose the correct model according to the symmetry onto which the strain is acting.



Strategy for Rietveld refinement

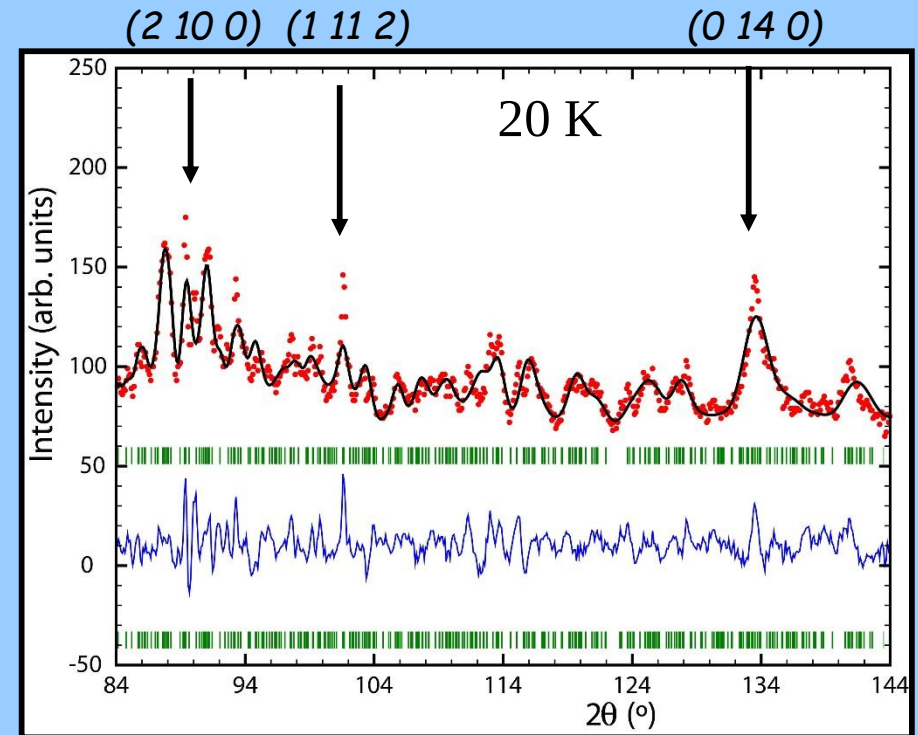
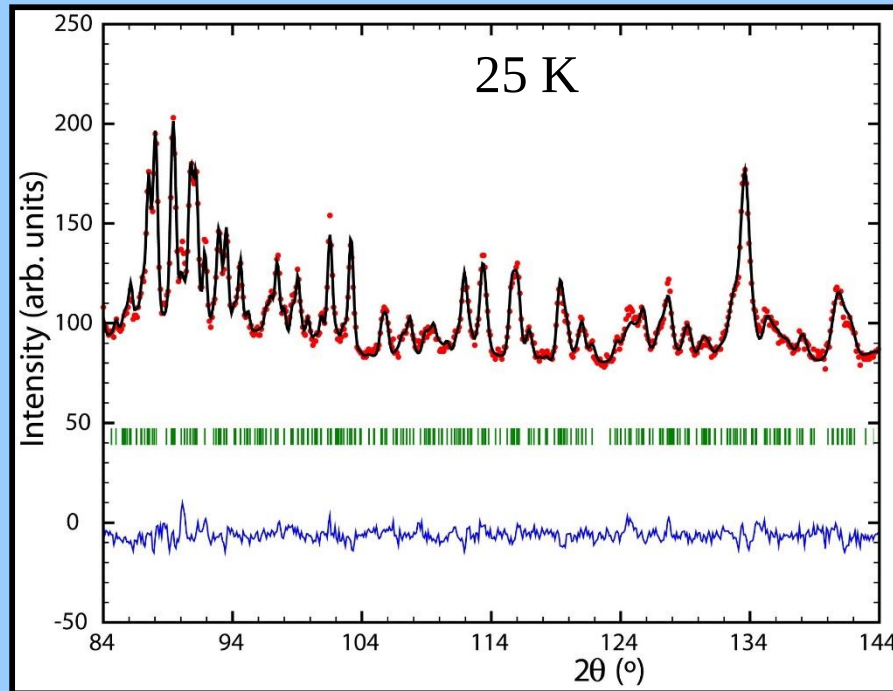
III) Some Selected Specific Problems:

2) Peak Shape:

Ho_5Ge_4 , magnetocaloric compound showing magnetostriction, orthorhombic structure:

Strong **anisotropic microstrain** appears as the Ho becomes magnetic

hkl dependence of peakwidth: peaks with large k are narrower



Use of the Stevens notation for the description of anisotropic strain

Needs the instrument resolution file as input!

```
!Job Npr Nph Nbg Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
1 7 2 34 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0
```

! Resolution file for Pattern# 1

New_D1A_191.irf

```
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
6 0 0 0.0 1.0 0.0 0 0 0 1 0 17501.770 0 7 0
```

Laue Class mmm

Strain-Model 3

!-----> Profile Parameters for Pattern # 1

```
! Scale Shape1 Bov Str1 Str2 Str3
0.50723E-01 0.00000 0.00000 0.00000 0.00000 0.00000
11.00000 0.000 0.000 0.000 0.000 0.000
```

```
! U V W X Y GauSiz LorSiz Size-Model
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0
0.000 0.000 0.000 0.000 0.000 0.000 0.000
```

```
! a b c alpha beta gamma #Cell Info
7.565165 14.560355 7.620977 90.000000 90.000000 90.000000
21.00000 31.00000 41.00000 0.00000 0.00000 0.00000
```

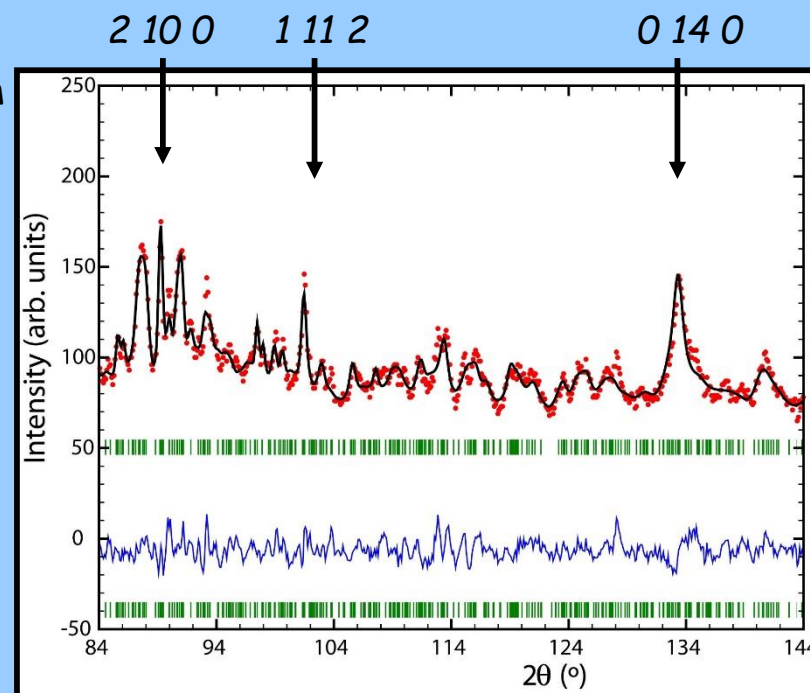
```
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
```

```
! S_400 S_040 S_004 S_220 S_202 S_022
0.180832 0.003863 0.043940 0.179977 20.769495 0.178759
141.00 161.00 121.00 131.00 111.00 311.00
```

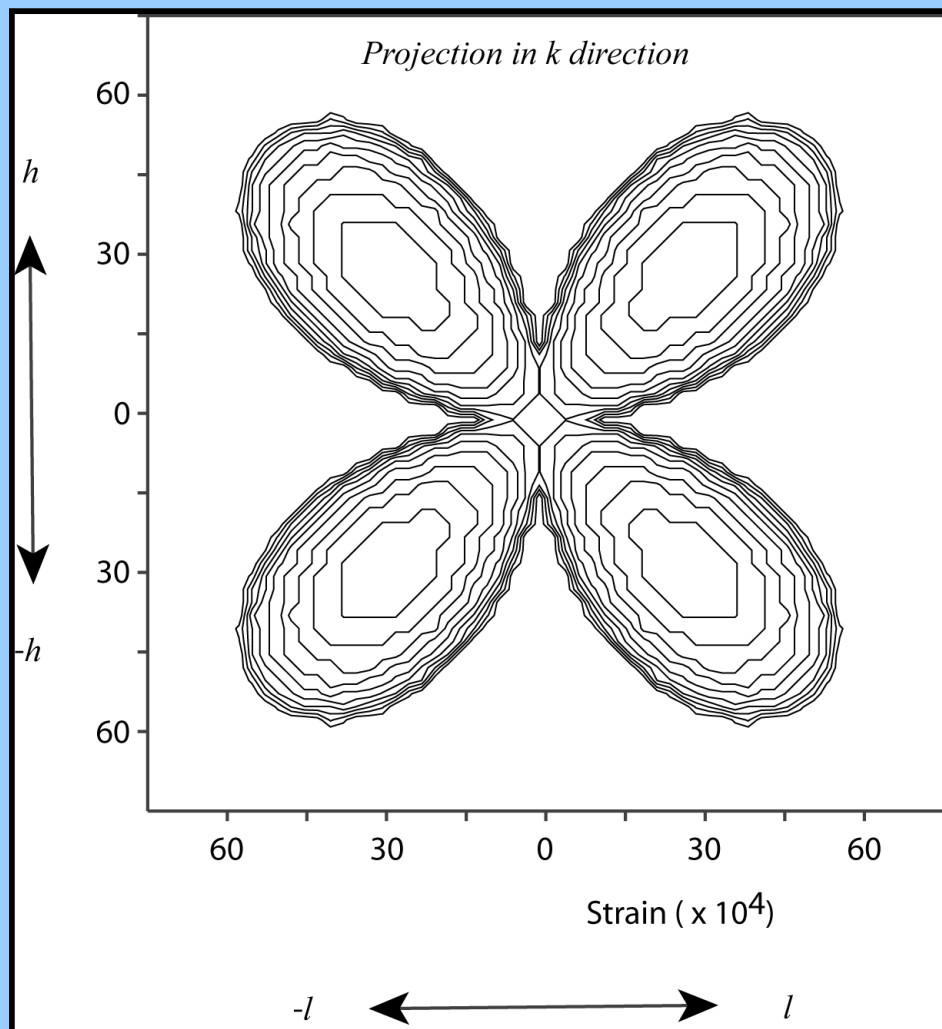
```
! Lorentzian strain coeff.+ code
0.17642 151.00000
```

Including anisotropic monoclinic strain:

Refinement a lot better but still not perfect



The patterns of microstrains can be visualized putting $J_{vi}=5$ in the PCR file (More=1) and reading the binary file with GFOURIER. Use projection mode.



Ho_5Ge_4

S_{202} is very large: strong tendency of the compound to switch to a monoclinic structure

Synchrotron data revealed later the real spacegroup: $P2_1/m$!

Microstructural parameters (see folder "Documents"):

$$H_{hG}^2 = (U_f + (1 - \xi_f)^2 D_{fST}^2(\alpha_D)) \tan^2 \theta + \frac{I_{fG}}{\cos^2 \theta} + H_{gG}^2$$

$$H_{hL} = (X_f + \xi_f D_{fST}(\alpha_D)) \tan \theta + \frac{[Y_f + F_f(\alpha_S)]}{\cos \theta} + H_{gL}$$

PCR Notation:

U_f = "U"	= Gaussian component of isotropic strain
X_f = "X"	= Lorentzian component of isotropic strain
I_{fg} = "GauSiz"	= Gaussian component of isotropic size
Y_f = "Y"	= Lorentzian component of isotropic size

D_{fST} , $F_f(\alpha_S)$ depend on the particular model chosen to describe anisotropic strain and size

D_{fST} in the Stevens Notation of anisotropic strain, up to 15 independent variables S_{hkl} with $(h+k+l)=4$

ξ = Mixing coefficient for Lorentzian contribution to anisotropic strain
= "Lorentzian strain coeff."

Lorentzian component to anisotropic size, depends on "Size-Model"
= "LorSiz "

Strategy for Rietveld refinement

IV) Constraints and restraints:

Applied in order to couple parameters so that they undergo the same linear or proportional shifts or to restrain parameters to stay within a given range.

1) Symmetry Constraints:

e.g.: Lattice parameters in a tetragonal system, code e.g.: 71.00 71.00 81.00

Atomic coordinates linked by symmetry e.g.:	$x, -x, z$, code e.g.: 101.00 -101.00 111.00
or:	$x, 2x, z$, code e.g.: 100.50 101.00 111.00

Scale factors of nuclear and magnetic phases having different unit cells,
with e.g.: $a\ b\ c$ (nuc) and $2a\ 2b\ c$ (mag): code 11.0000 (nuc) and 10.0625 (mag)

Refining a low symmetric structure with limited data (forcing e.g. part of a framework of atoms to keep a higher symmetry, e.g.: charge ordered structures with Mn^{3+} and Mn^{4+} in $Tb_{0.5}Ca_{0.5}MnO_3$:

$Pnma$ with $a\ b\ c$ has 7 positional parameters,

$P2_1/m$ with $2a\ b\ c$ has 31 positional parameters. **Nowadays: Use Amplitudes to refine distortions**

Spin direction in highly symmetric cases, e.g.: hexagonal system: refine only M_x and M_z as powder data don't allow the determination of the moment direction within the basal plane.

Strategy for Rietveld refinement

IV) Constraints and restraints:

2) Constraints due to direct correlation, e.g.:

Wavelength or lattice parameters (refine one or the other)

Scale factor or magnetic moment value in a purely magnetic phase (using a difference data set)

Scale factor and site occupancies (has to be fixed for one site)

General Remark 1:

Put **Ana = 1** in pcr file for analysis of Refinement:

Pay attention to message "Correlation of special kind" indicates coupling of strongly correlated = wrongly coupled parameters.

General Remark 2:

Some correlations are very strong, e.g.: zero shift and sample displacement.

This will increase your standard deviations. If interested in relative behaviour of parameters as function of e.g. T keep some fixed.

General Remark 3:

When you do a **sequential refinement** using data from a stationary multidetector (e.g. D20, D1B) you refine only once the **zeroshift** using one data set and then you **fix** it.

Strategy for Rietveld refinement

IV) Constraints and restraints:

3) Linear Restraints:

E.g.: Partial site occupancies (total must be fixed, not negative, with several sites ...)

		x	y	z	B	Occ				
CR	CR	0.00000	0.00000	0.00000	0.00000	0.01563	0	0	0	2
		0.00	0.00	0.00	0.00	211.00				
RE	RE	0.00000	0.00000	0.00000	0.00000	0.00190	0	0	0	3
		0.00	0.00	0.00	0.00	221.00				
FE	FE	0.00000	0.00000	0.00000	0.00000	0.00331	0	0	0	3
		0.00	0.00	0.00	0.00	271.00				
RE	RE	0.50000	0.50000	0.50000	0.00000	0.01372	0	0	0	3
		0.00	0.00	0.00	0.00	231.00				
FE	FE	0.50000	0.50000	0.50000	0.00000	0.00190	0	0	0	3
		0.00	0.00	0.00	0.00	281.00				
CR	CR	0.50000	0.50000	0.50000	0.00000	0.00520	0	0	0	2
		0.00	0.00	0.00	0.00	241.00				

Occupation of site =

Site Multiplicity/ Multiplicity of the general site
Fm3m: 4/192 = 0.02083 if full

Site 1

$\text{Sr}_2\text{CrFe}_{0.25}\text{Re}_{0.75}\text{O}_6$ with Cr, Fe and Re distributed over 2 cation sites (4a: 0 0 0 and 4b: $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$):

Site 2

Introduce linear restraints, NLI in pcr file, **NLI = 5** (second line of pcr-file)

! Set of 5 linear restraints:

! Identifier, number of coeff., value, sigma / List of coeff & Parameters

Site_a 3 0.020830 0.0000001
1.0000 21 1.0000 22 1.0000 27
(Limits the occupation on site 0 0 0 to 0.02083 = FULL)

Site_b 3 0.020830 0.0000001
1.0000 23 1.0000 24 1.0000 28
(Limits the occupation on site $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ to 0.02083 = FULL)

Chemcomp 2 0.020830 0.0000001
1.0000 21 1.0000 24
(Limits the total content of Cr on both sites to 0.02083 = 1)

Chemcomp 2 0.015620 0.0000001
1.0000 22 1.0000 23
(Limits the total content of Re on both sites to 0.01562 = 0.75)

Chemcomp 2 0.005210 0.0000001
1.0000 27 1.0000 28
(Limits the total content of Fe on both sites to 0.00521 = 0.25)

Constraint pcr

Fp

Strategy for Rietveld refinement

IV) Constraints and restraints:

- 4) 'Strategic' Constraints: Used in order to assure a successful refinement
(can be lifted as the refinement proceeds)

In theory not needed if the data would be perfect in intensity, resolution and q-range.

In powder always limitations: Same q-value for different reflections (5 5 3, 7 1 1 in cubic system)
Multiplicity of reflections (311, 131, 113...)

Typical 'strategic' constraints:

One overall temperature factor for all atoms

The same temperature factor for all atoms of the same type

Magnetic moment values of different magnetic sites kept alike

Limit the possible Spin directions (basis vectors)

Refining a magnetic structure using high intensity/low resolution data:

Keep all atom coordinates fixed if the crystallographic structure had been determined before from high resolution data.

Again: Keep the zeroshift fixed in a sequential refinement!!

Strategy for Rietveld refinement

IV) Constraints and restraints:

- 5) Restraints: Helps the refinement program not to get trapped in false minima
Very important for e.g. simulated annealing

P 21/n		<--Space group symbol								
!Atom Typ	X	Y	Z	Biso	Occ	In Fin	N_t	Spc	/Codes	
Sr SR	0.87930	0.41798	0.73560	1.55853	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
C1 C	0.63200	0.23920	0.57800	1.48511	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
C2 C	0.58300	0.51640	0.09300	1.48511	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
C3 C	0.64800	0.27780	0.34700	1.48511	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
O1 O	0.62200	0.22870	0.15700	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
O2 O	0.67300	0.28130	0.75600	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
Ow3 O	0.85600	0.56610	0.57600	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
O4 O	0.77900	0.50850	0.07000	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
O5 O	0.57500	0.16760	0.56900	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
O6 O	0.52400	0.55480	0.26500	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
O7 O	0.69400	0.34880	0.32900	1.24468	1.00000	0	0	0	0	0
	0.00	0.00	0.00	0.00	0.00					
H1 D	0.77449	0.06512	0.01765	2.00000	1.00000	0	0	0	0	0
	11.00	21.00	31.00	0.00	0.00					
H2 D	0.81474	0.75317	0.49374	2.00000	1.00000	0	0	0	0	0
	41.00	51.00	61.00	0.00	0.00					
H3 D	0.64942	0.10371	0.81023	2.00000	1.00000	0	0	0	0	0
	71.00	81.00	91.00	0.00	0.00					

Strontium-Oxalate (deuterated)

Where is the Hydrogen?

Keep the known framework fixed

Coordinates of 3 H atoms free

NRE in pcr file = number of restraints

Put NRE = 9 (first line of pcr-file)

Nine Restraints to be put into the pcr-file:

! Limits for selected parameters (+ steps & BoundCond for SA):

1	0.0000	1.0000	0.0152	1	X_H1
2	0.0000	1.0000	0.0073	1	Y_H1
3	0.0000	1.0000	0.0264	1	Z_H1
4	0.0000	1.0000	0.0279	1	X_H2
5	0.0000	1.0000	0.0080	1	Y_H2
6	0.0000	1.0000	0.0323	1	Z_H2
7	0.0000	1.0000	0.0334	1	X_H3
8	0.0000	1.0000	0.0087	1	Y_H3
9	0.0000	1.0000	0.0346	1	Z_H3

Strategy for Rietveld refinement

IV) Constraints and restraints:

6) Soft distance (or angles) constraints

Running Fullprof with the option of calculating distances and angles (**Jdi = 3, needs More=1 in line starting with Nat**) will not only produce a file called *.dis with all the interatomic distances and angles, but as well a file called **CFML_Restraints.tpcr**.

```
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
  7  0  0  0.0 0.0 1.0  0  0  0  0  0  967.370  0  5  1
!Jvi Jdi Hel Sol Mom Ter Brind RMua RMub RMuc Jtyp Nsp_Ref Ph_Shift N_Domains
  0  3  0  0  0  0  1.0000 0.0000 0.0000 0.0000  1  0  0  0
! Max_dst(dist) (angles) Bond-Valence Calc.
   3.6000   2.6000   BVS
! N_cations N_anions Tolerance(%) / Name or cations/ and Anions
   3         1       0.00
PR+3 FE+3 B3+
O-2
```

pcr file

CFML_Restraints.tpcr

YFe3BO34disconstraints.pcr

Fp

YFe3BO34disconstraints.dis

This file contains in the appropriate format distance or angle restraints which can be pasted into the pcr file.
This is useful if you want to restrain a certain type of interatomic distances (or angles) to be the same

=> Help for possible angle restraints around atom FE2

FE2	O2	O2	32	33	0.0000	-1.0000	0.6667	-1.0000	-1.0000	0.3333	46.36	0.18
FE2	O2	O4	32	25	0.0000	-1.0000	0.6667	0.0000	0.0000	0.0000	5.53	0.18
FE2	O2	O5	32	26	0.0000	-1.0000	0.6667	0.0000	-1.0000	0.3333	41.58	0.24
FE2	O2	O5	32	27	0.0000	-1.0000	0.6667	0.0000	0.0000	0.6667	51.04	0.24

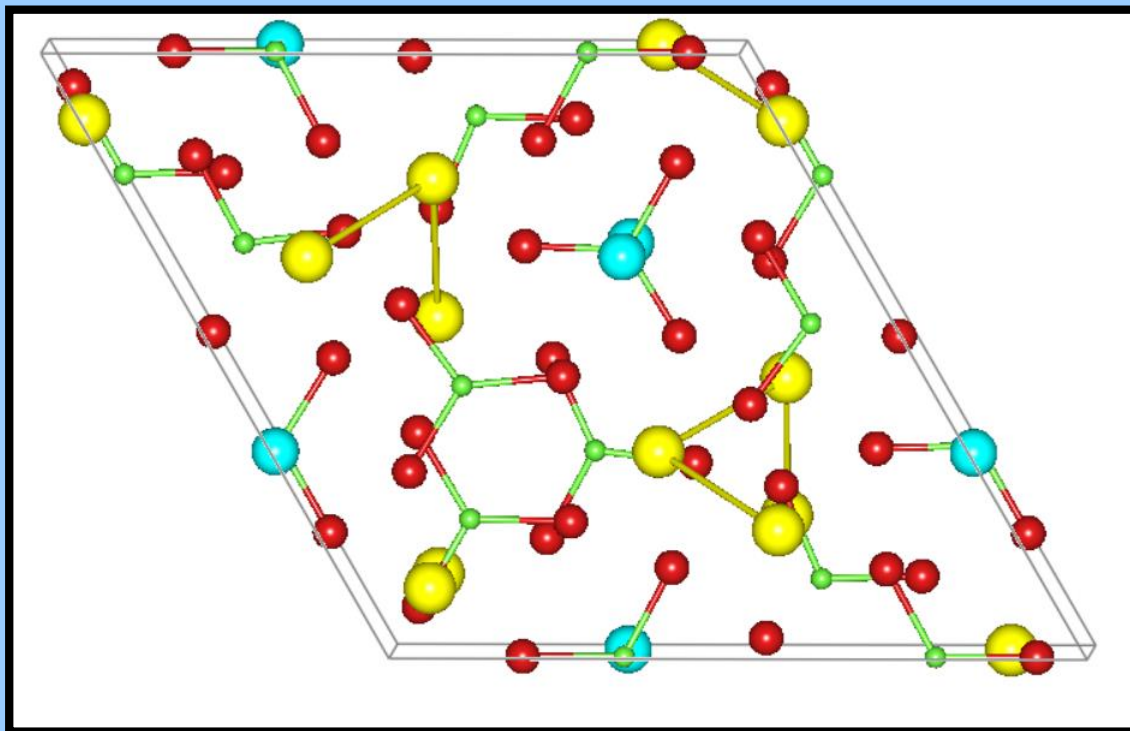
At1	At2	ITnum	T1	T2	T3	DIST	SIGMA
FE2	FE2	26	-1.00000	-1.00000	0.33333	3.1853	0.0049
FE2	FE2	27	0.00000	-1.00000	-0.33333	3.1853	0.0044
FE2	FE2	33	0.00000	0.00000	0.33333	4.4180	0.0053
FE2	Y	25	0.00000	0.00000	0.00000	3.8107	0.0073

In the pcr file you have to change as well the parameters **DIS** or **MOM** to the number of restraints you introduced.

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6) Soft distance (or angles) constraints



Example of $\text{YFe}_3(\text{BO}_3)_4$:
Groups of BO_3

$$R_{\text{Bragg}} = 3.7$$

unconstrained

$$R_{\text{Bragg}} = 3.9$$

B-O distances constrained to be equal

Thank you for your attention!