Refinement of Crystallographic and Magnetic Structure of $CaMnO_3$ Using HIPD

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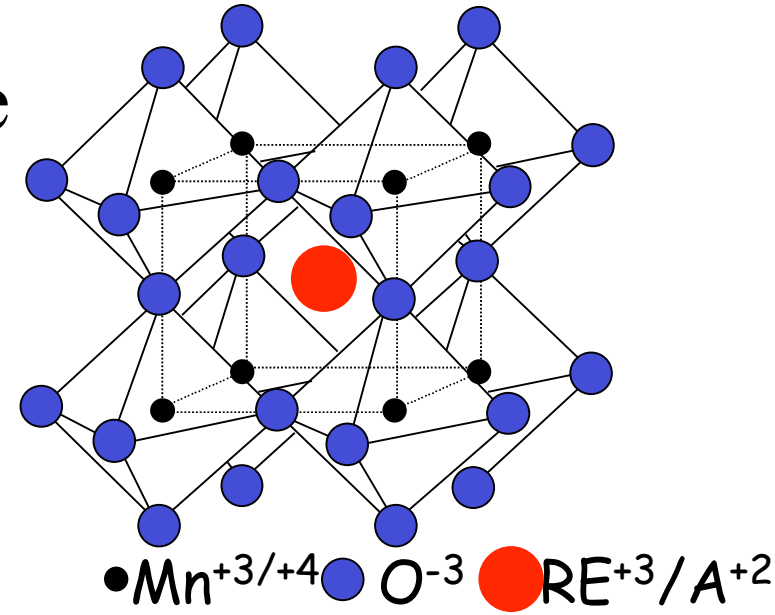
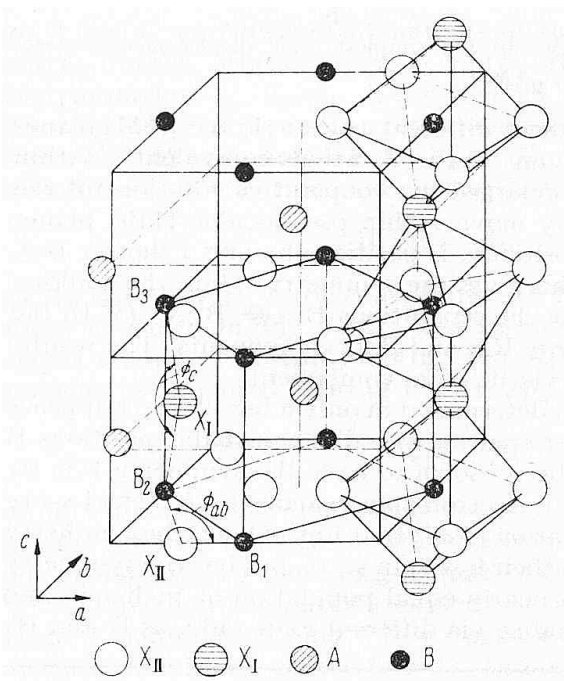
Outline

- Introduction
- Experiment
- Results
- Discussion
- Conclusions

Introduction

- Determine magnetic structure of the Perovskite $CaMnO_3$

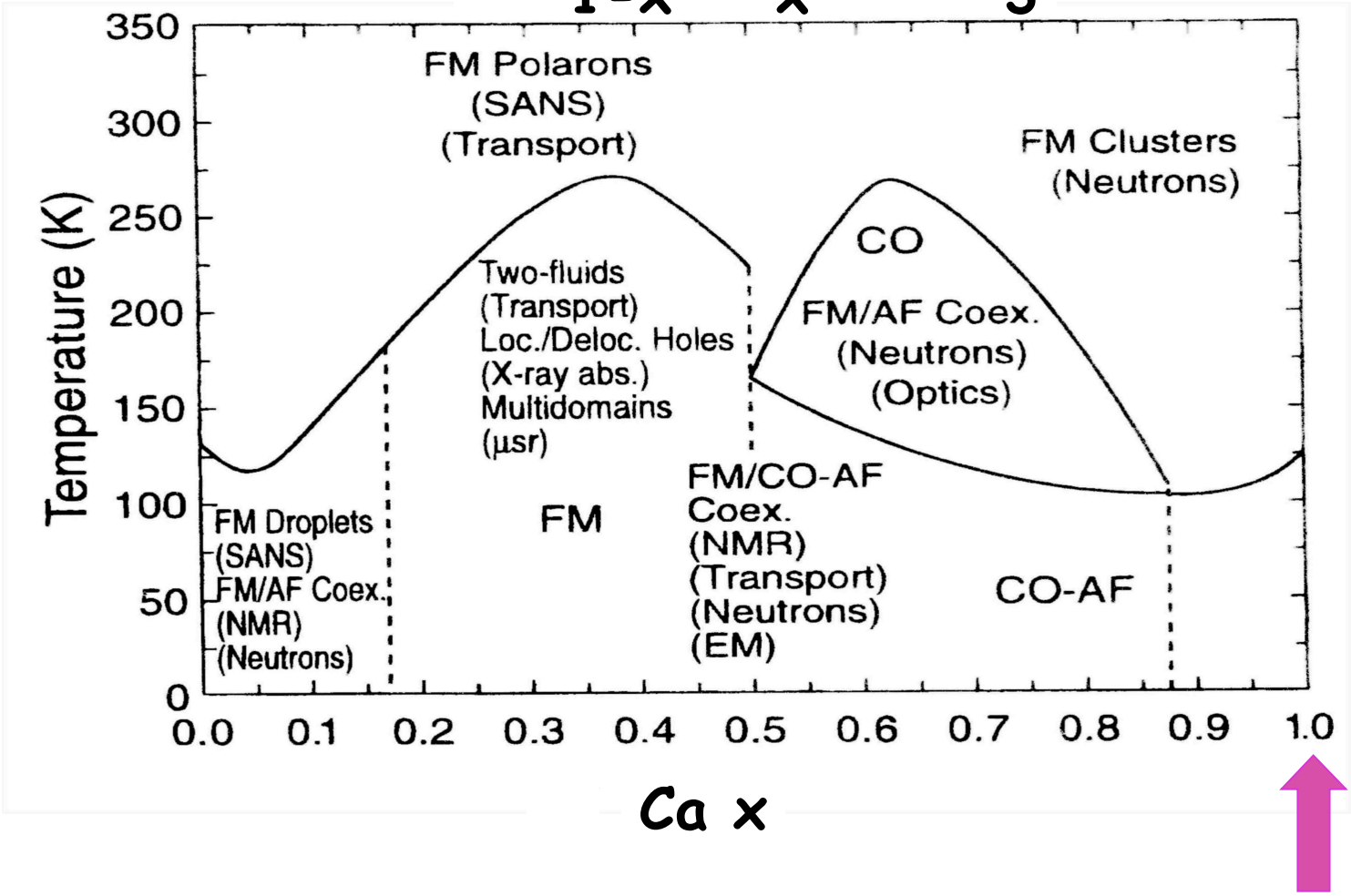




Sp. Grp. *Pbnm*

a	5.454729	b	5.451733	c	7.697468		
α	90.0000	β	90.0000	γ	90.0000		
CA	CA+2	0	0	0	0.981722	0.026560	0.250000
MN	MN	0	0	0	0.000000	0.500000	0.000000
O4	O-2	0	0	0	0.065289	0.496088	0.250000
O5	O-2	0	0	0	0.721105	0.276173	0.028997

$La_{1-x}Ca_xMnO_3$



$CaMnO_3$ – AF; T_N = ~125 K

Diffraction: elastic scattering

-Braggs law: $\lambda = 2d\sin(\theta)$

$$\lambda = \frac{h}{mv} = \frac{ht}{mL}$$

TOF

$$d = \frac{h\,t}{2\,m\,L\sin(\theta)}$$

-L, θ determined by the instrument

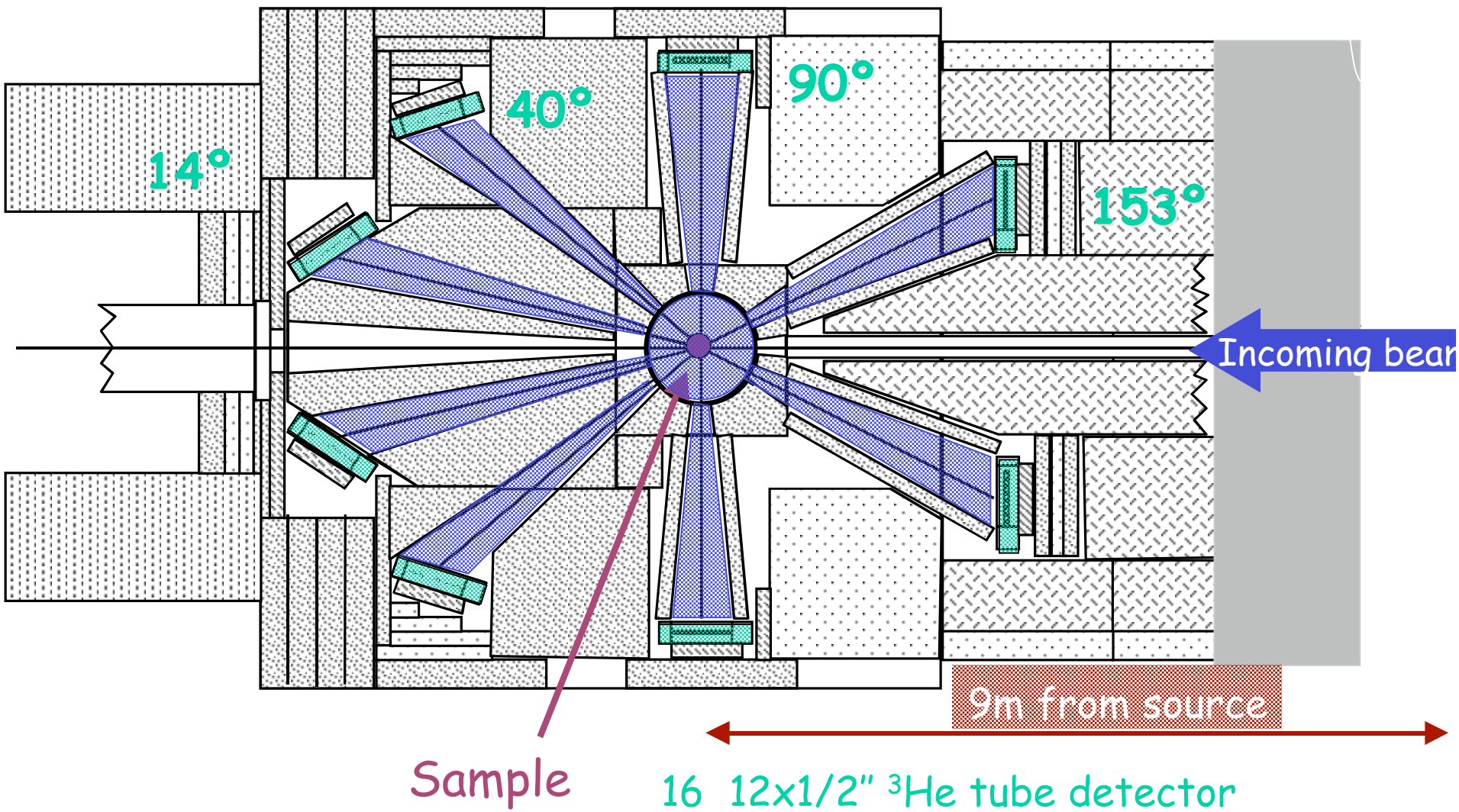
-In TOF measure *t*

$$\lambda = \frac{h}{mv}$$

$$v = \frac{L(\text{distance from choper to detector})}{t(\text{time taken})}$$

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta t}{t} = \frac{\Delta t}{L}\frac{h}{m\lambda} = \frac{\Delta t}{L}\frac{h}{2md\sin\theta}$$

Introduction: HIPD



Experiment

- Collect powder diffraction data using HIPD at two temperatures T = 300 K and T= 20 K
- Data acquired in 8 detector banks in one hour at both temperatures

Diffraction data
Hystogram I(time)
Parameters
instrument

datafile.gsas

instrument.iparm

GSAS FLOWCHART

1-EXPGUI
Simple editor for .exp file
Graphical interface
1'-EXPEDIT
Full expfile.EXP editor
Command line

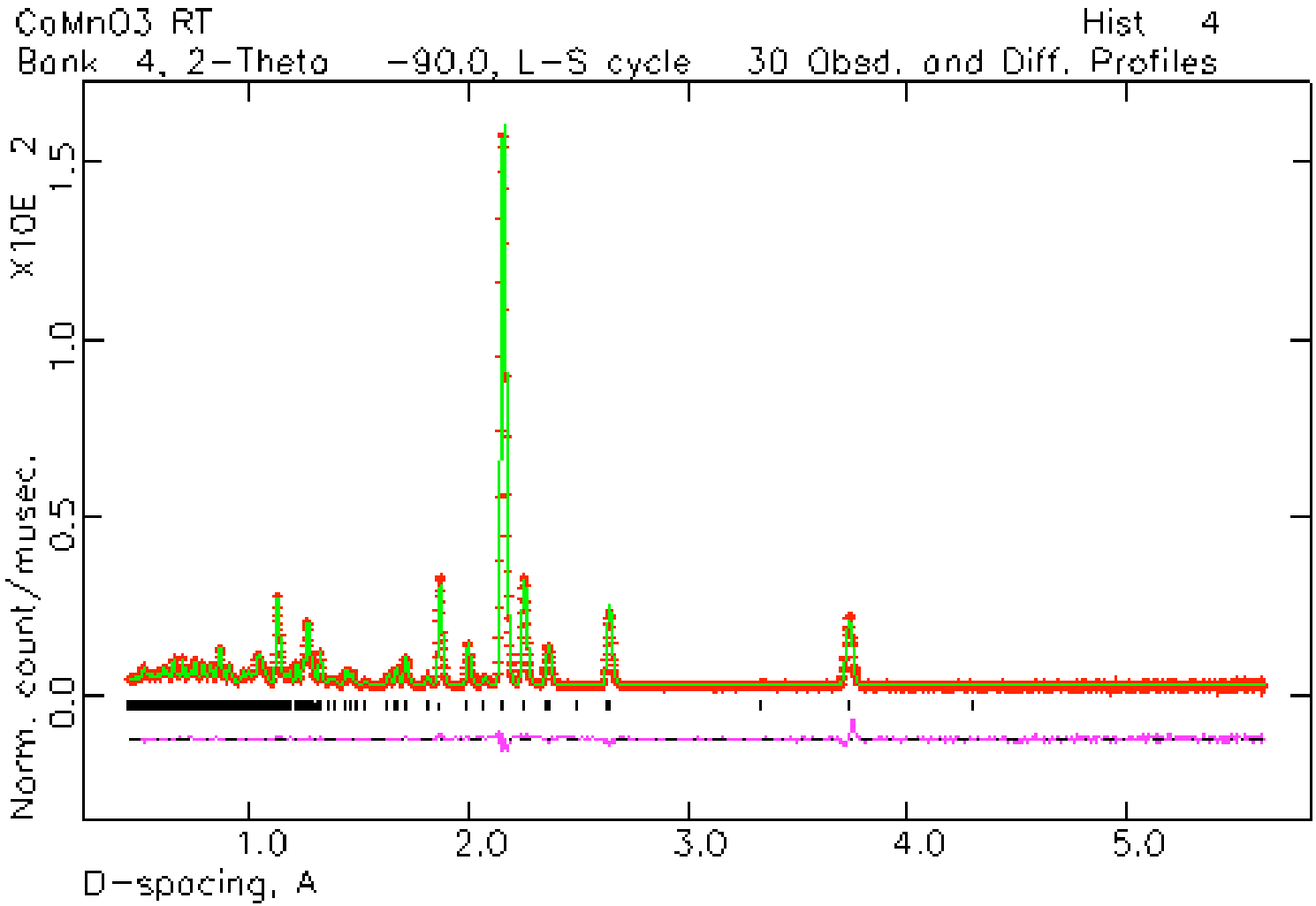
GSAS
Experiment file
expfile.EXP

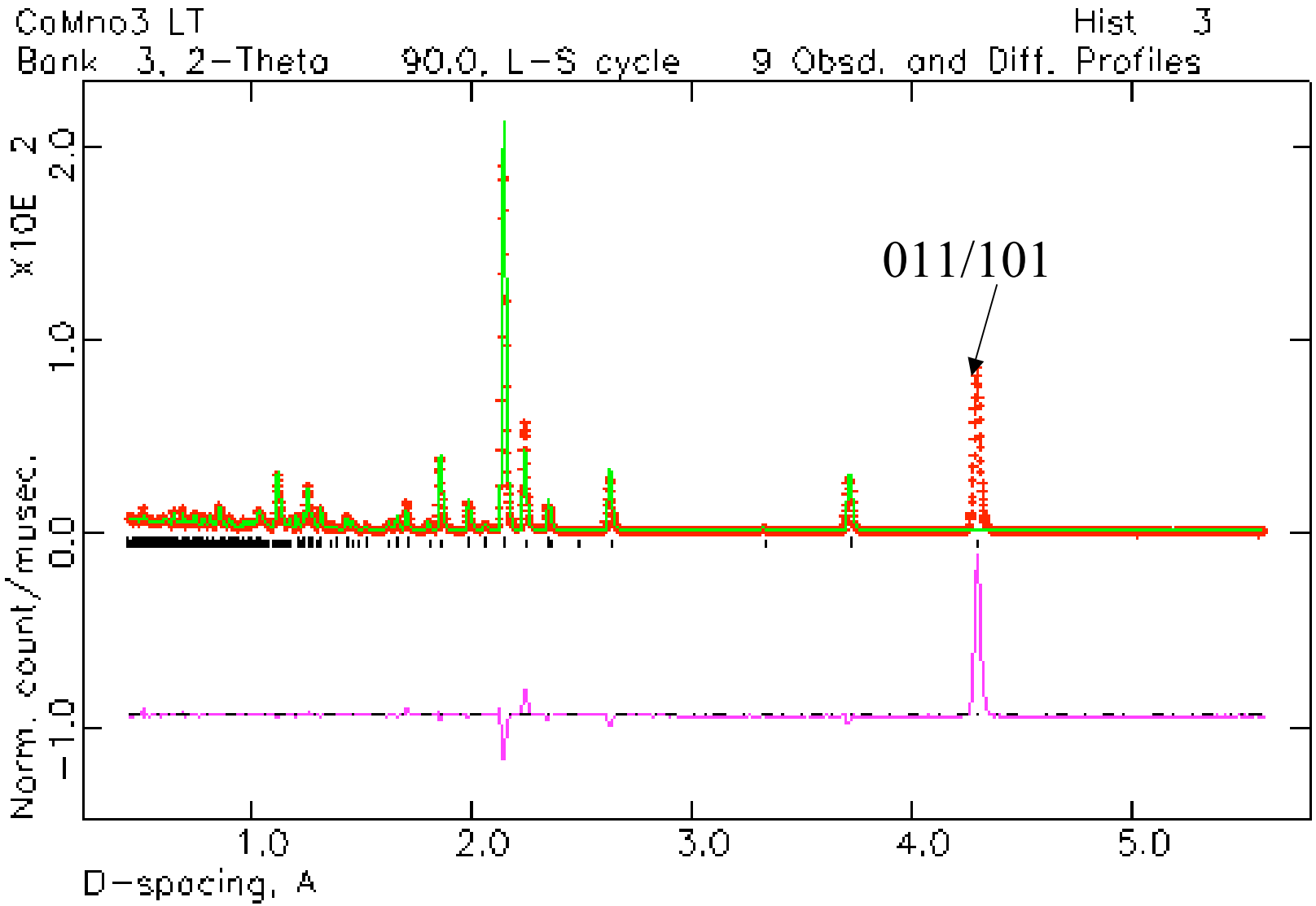
3-GENLES
(least squares)

Expfile.lst
Listing file

2-POWPREF
Generates the reflections

Data: Room Temperature



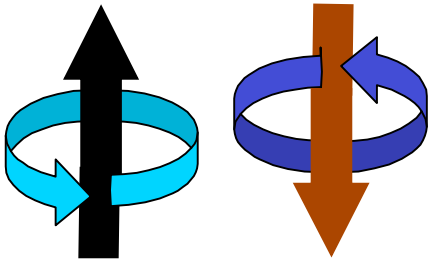


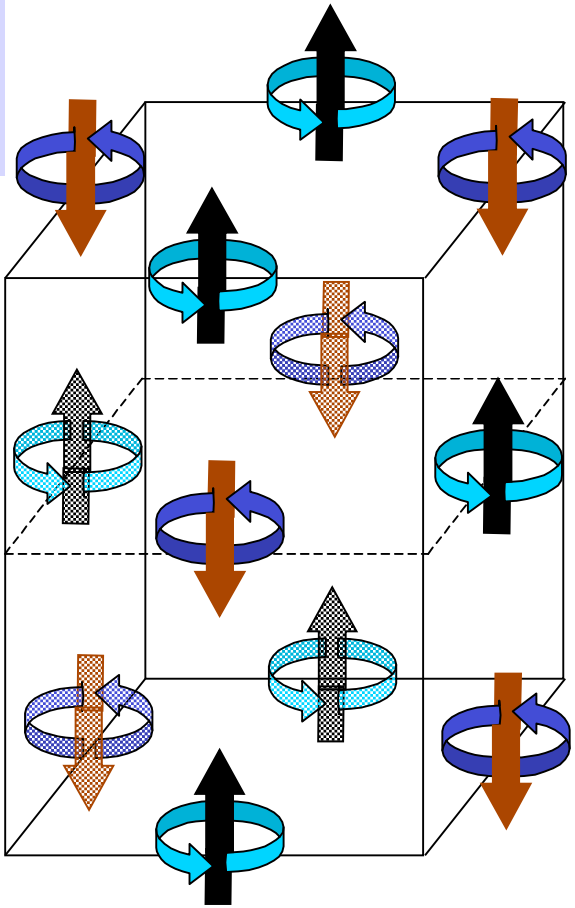
T = 20K, refined using only nuclear structure model from T = 300 K

Model

Space group: P b n m

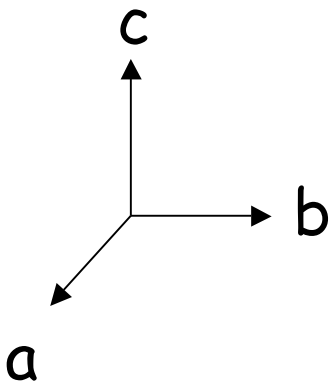
- P → Primitive orthorhombic lattice
- b → Glide plane _ a-direction
- n → Glide plane _ b-direction
- m → Mirror plane _ c-direction





The possibilities

Pbnm	Pb'nm
Pb'n'm'	Pb'n'm
Pbnm'	Pbn'm'
Pbn'm	Pb'nm'



Model

Which one works?

Pbnm

Pb'nm

Pb'n'm'

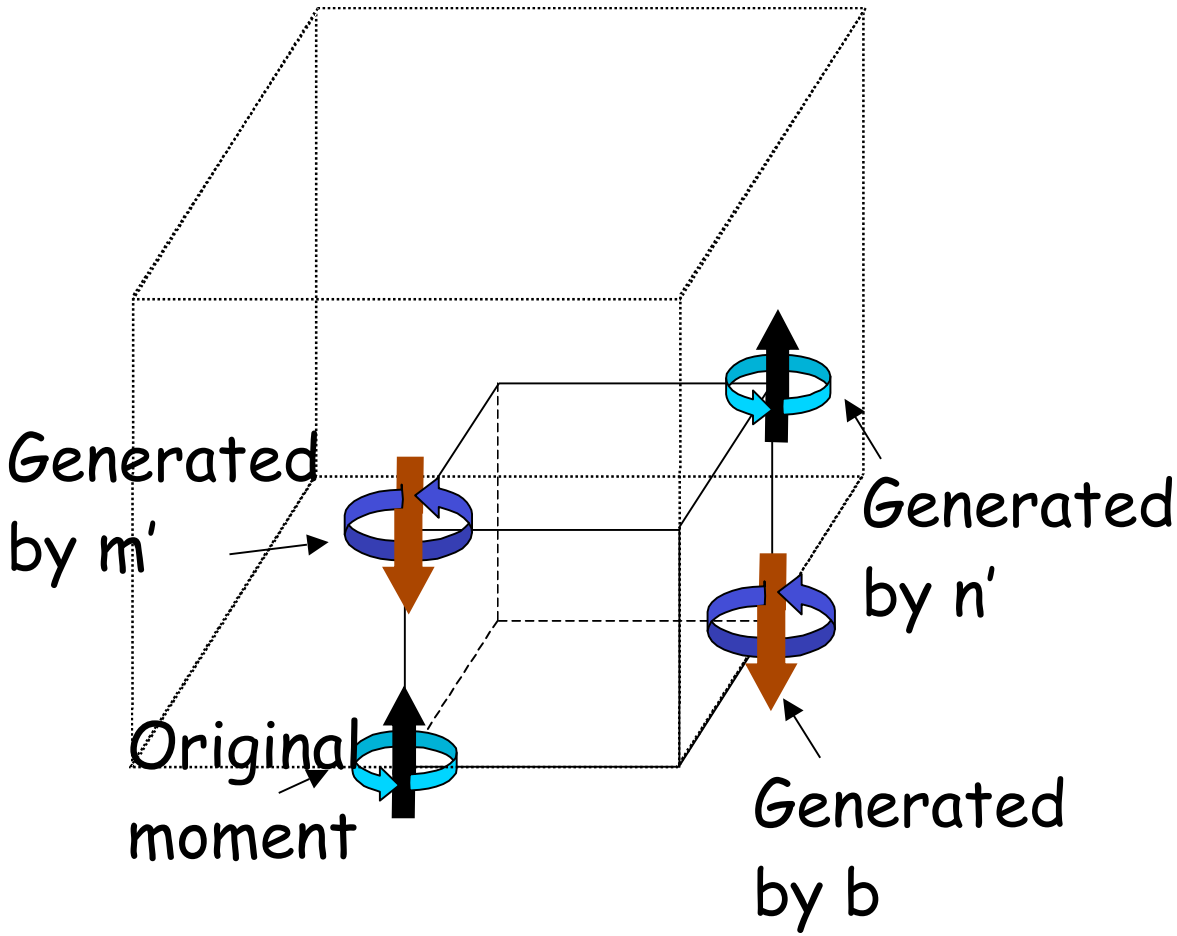
Pb'n'm

Pbnm'

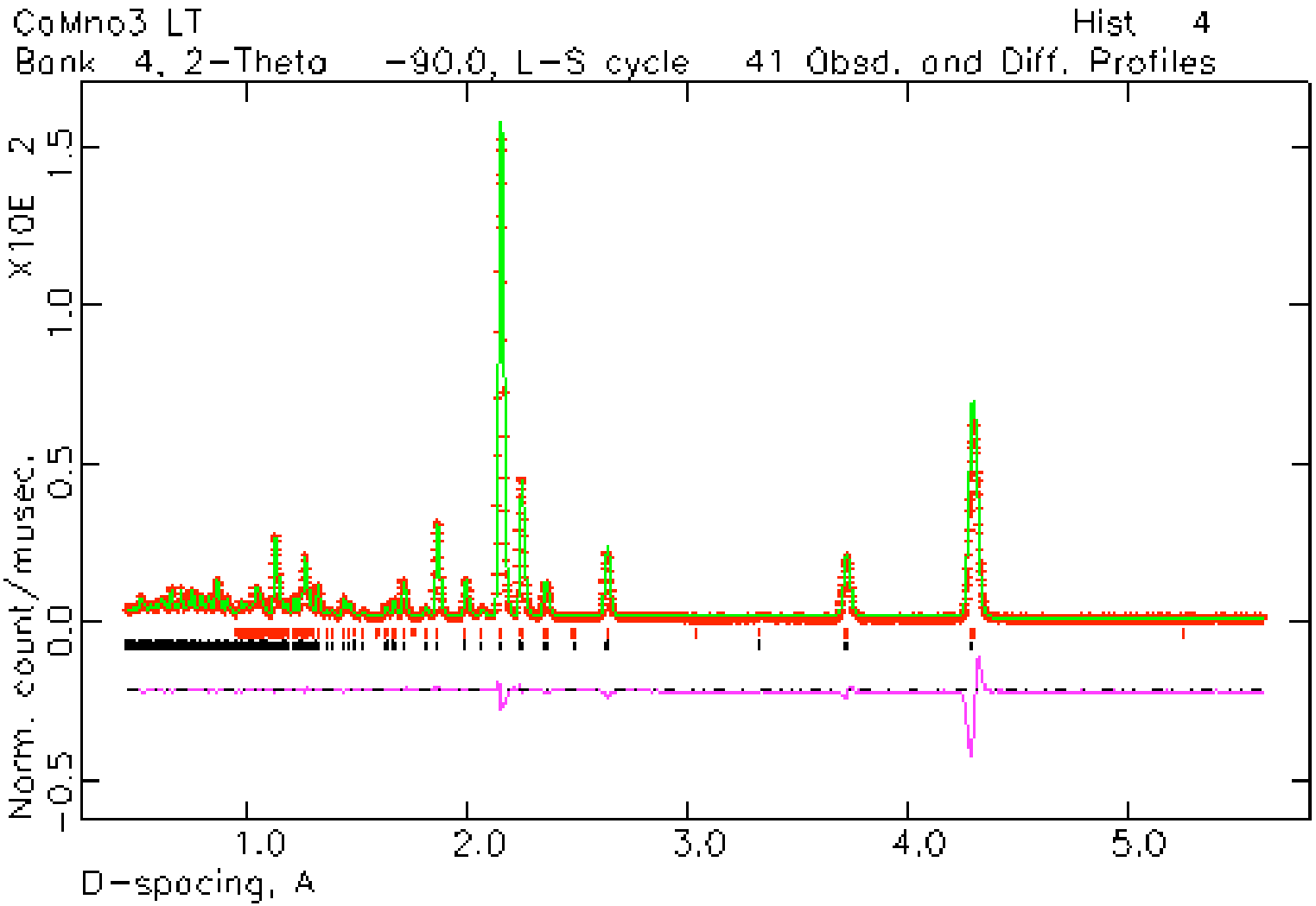
Pbn'm'

Pbn'm

Pb'nm'



- After seeing the difference, magnetic peaks were refined separately



Results

Mz (ì÷	T = 300 K	T = 20 K
Mn-O1 (□2) (Å)	1.89620(12)	1.89004(4)
Mn-O2 (□2) (Å)	1.9015(5)	1.89866(2)
Mn-O2 (□2) (Å)	1.9075(5)	1.90162(2)
B)	-	2.511(3)
2	4.2	16.9
R_{wp} (%)	3.5	4.4

- Observe slight shortening of Mn-O bond lengths with a decrease in temperature
- AFM contribution from M_z= 2.5□□

Conclusions

- Crystal and magnetic structure of $CaMnO_3$ determined using Rietveld refinement
- Crystal and magnetic structure have same unit cell
- Magnetic structure is AF, $M_z = 2.5$ _B

Acknowledgements

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