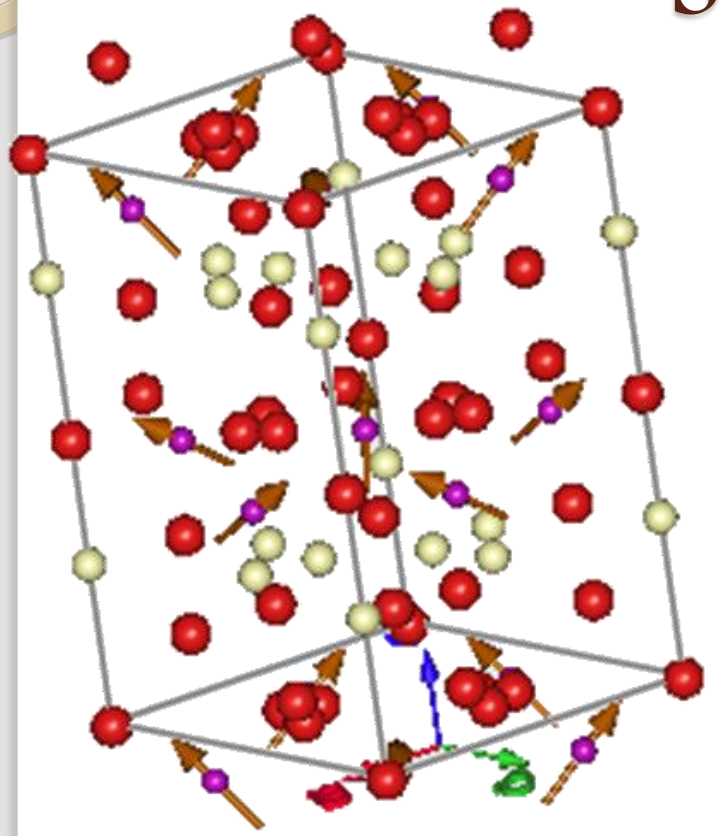
Crystal and Magnetic Structure of $LuFeO_3$



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Sang W. Cheong
Jeff Lynn
William Ratcliff

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NIST Center for Neutron Research

RUTGERS

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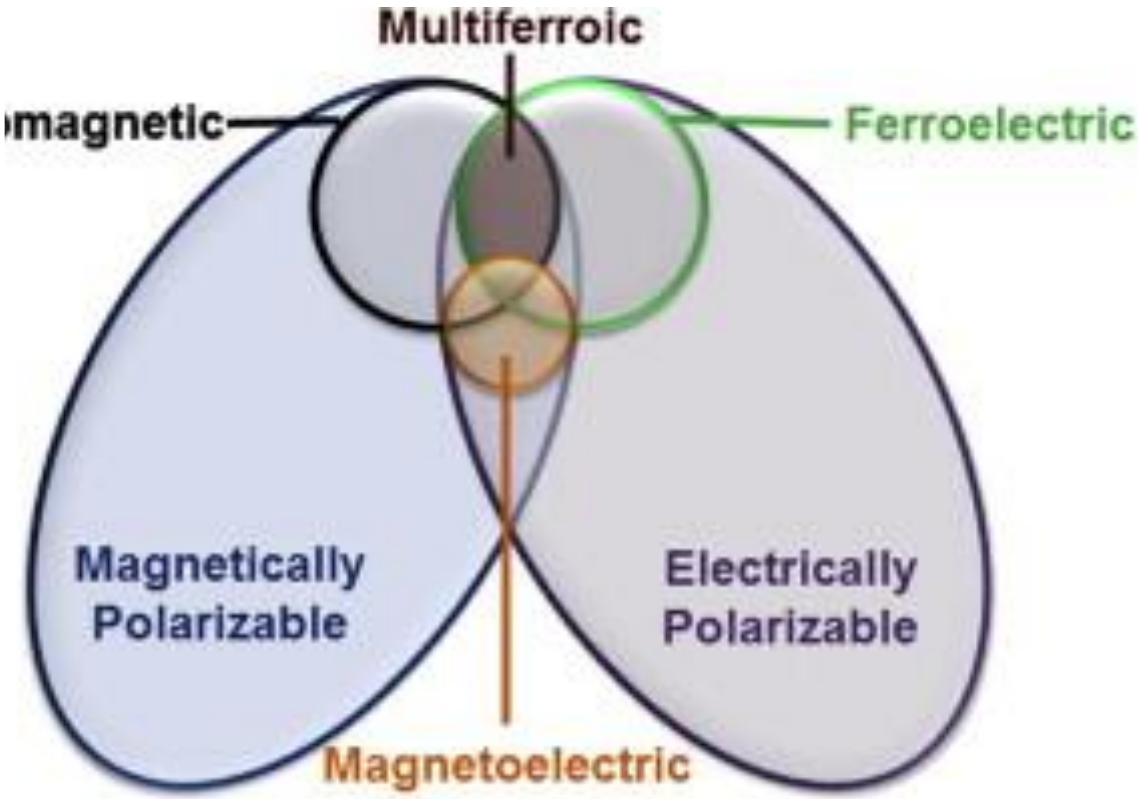
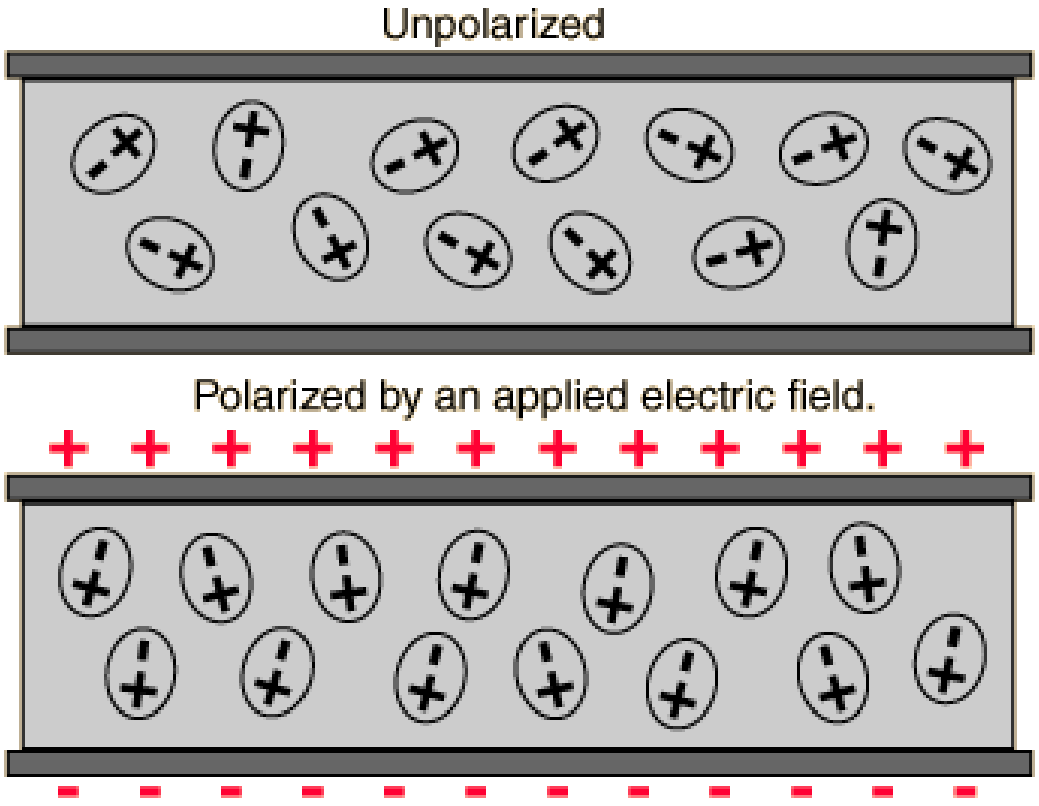
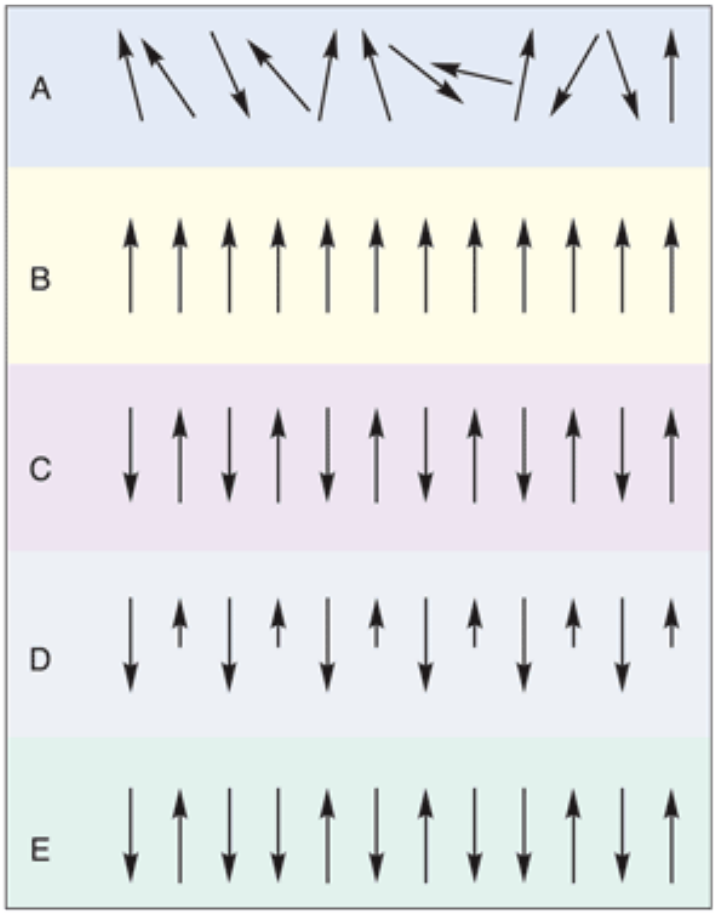
CRESCENS SCIENTIA

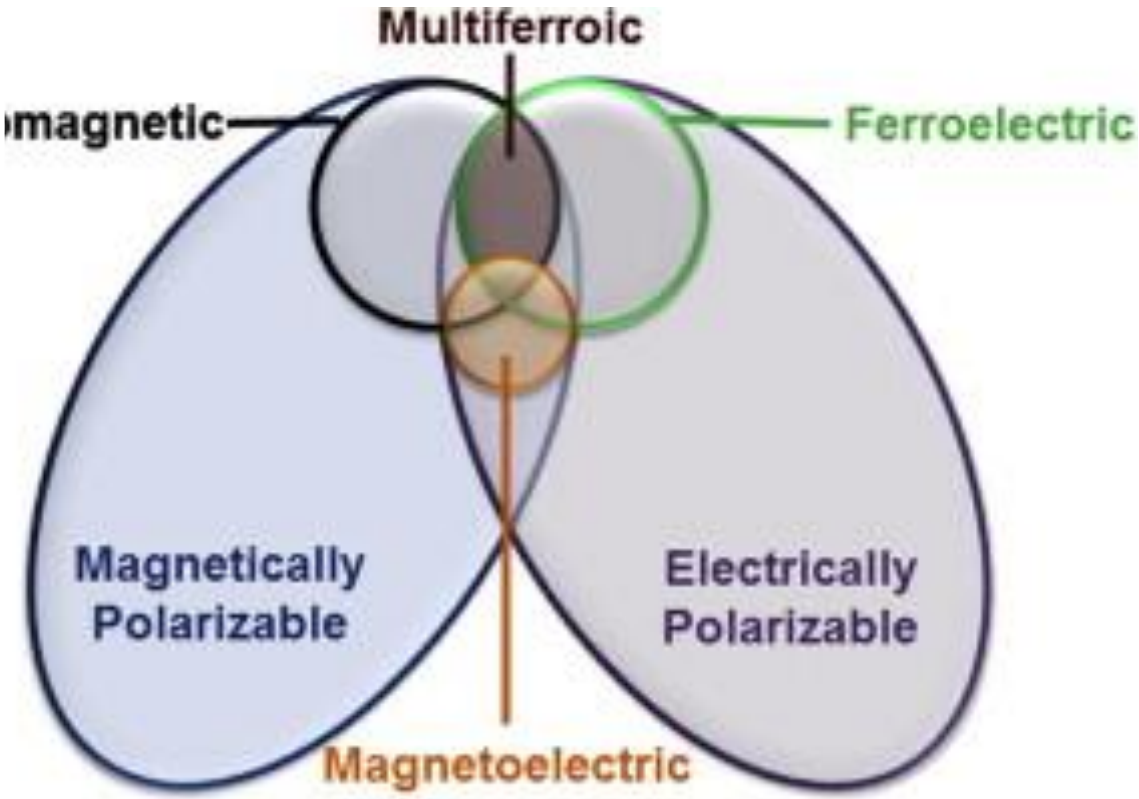

Multiferroic
magnetic
Ferroelectric
Magnetically
Polarizable
Electrically
Polarizable
Magnetoelectric

Ferroelectric



Magnetism



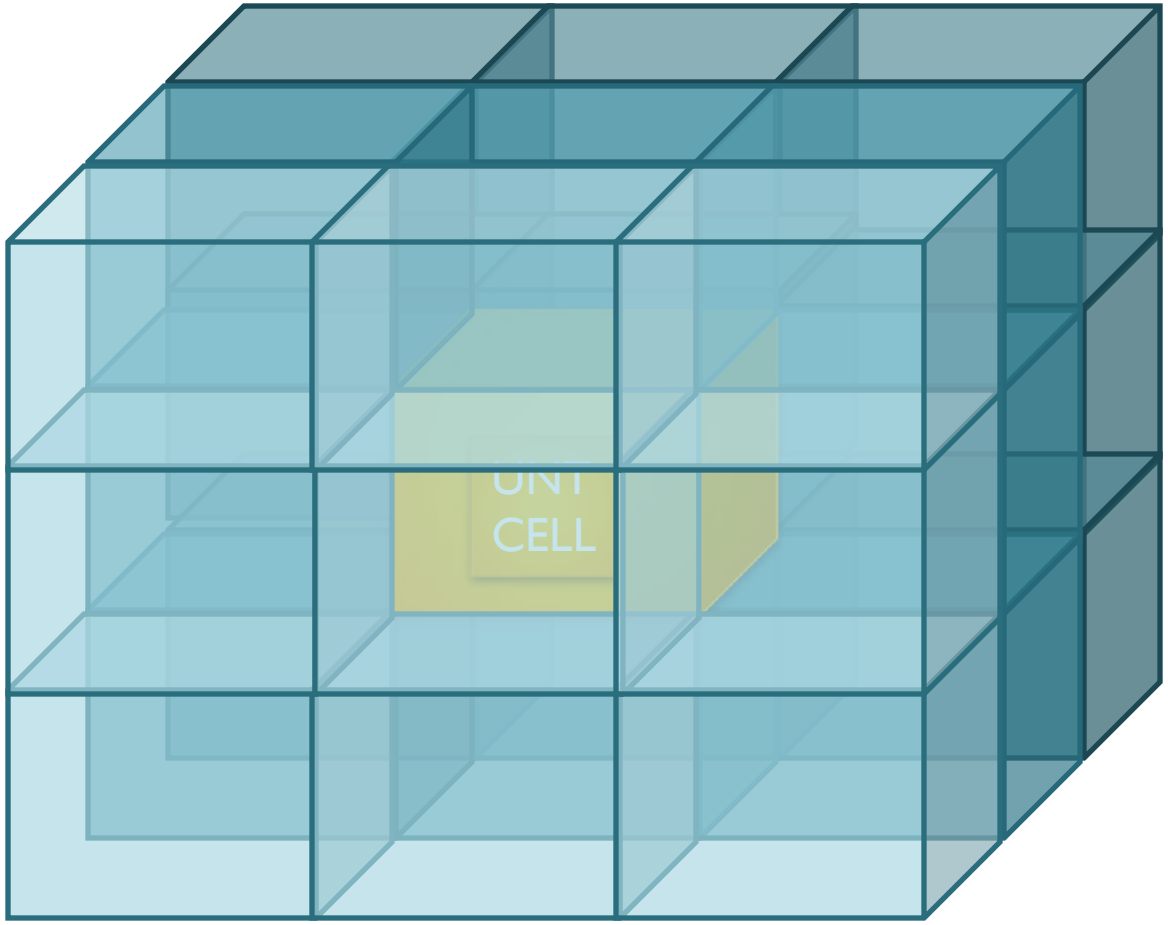

Multiferroic
magnetic
Ferroelectric
Magnetically
Polarizable
Electrically
Polarizable
Magnetoelectric

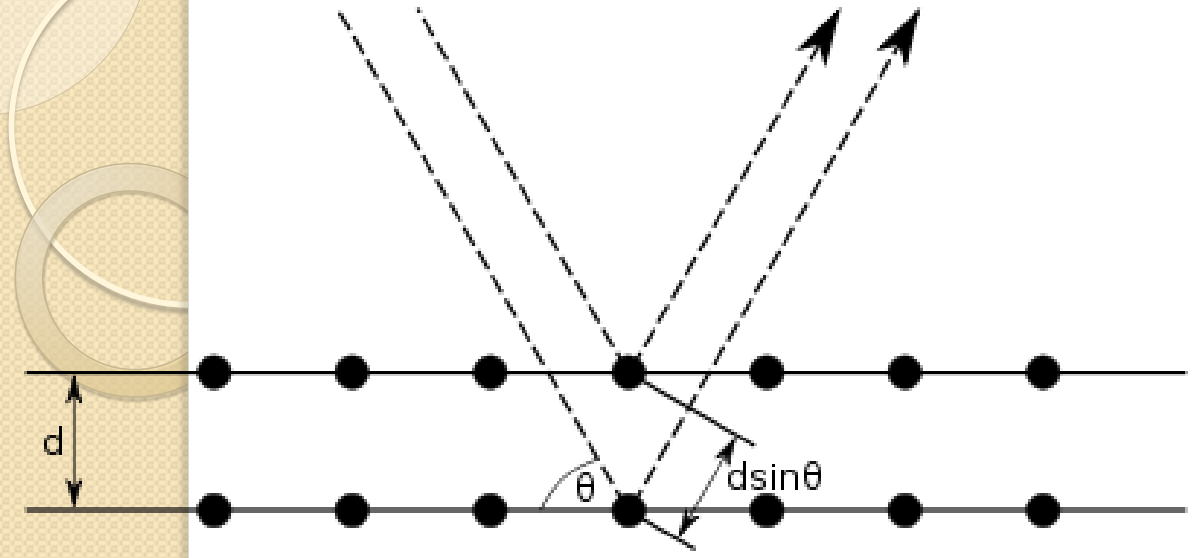
$LuFeO_3$

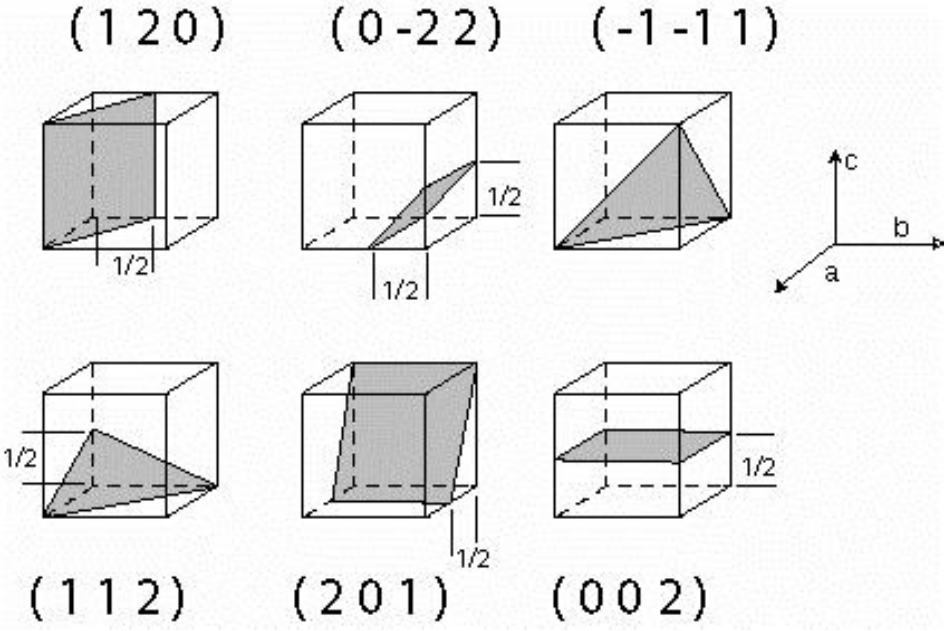
- $LuFe_{.75}Mn_{.25}O_3$
- T_{Curie} : ~1050K
  - Controversial discovery by ORNL[1]
    - T_{Neel} : ~440K
  - What it should be (following $YMnO_3$, $HoMnO_3$)
    - T_{Neel} : ~130K

[1] Wenbin Wang et al., Phys Rev. Lett 110, 237601 (2013)

Crystals

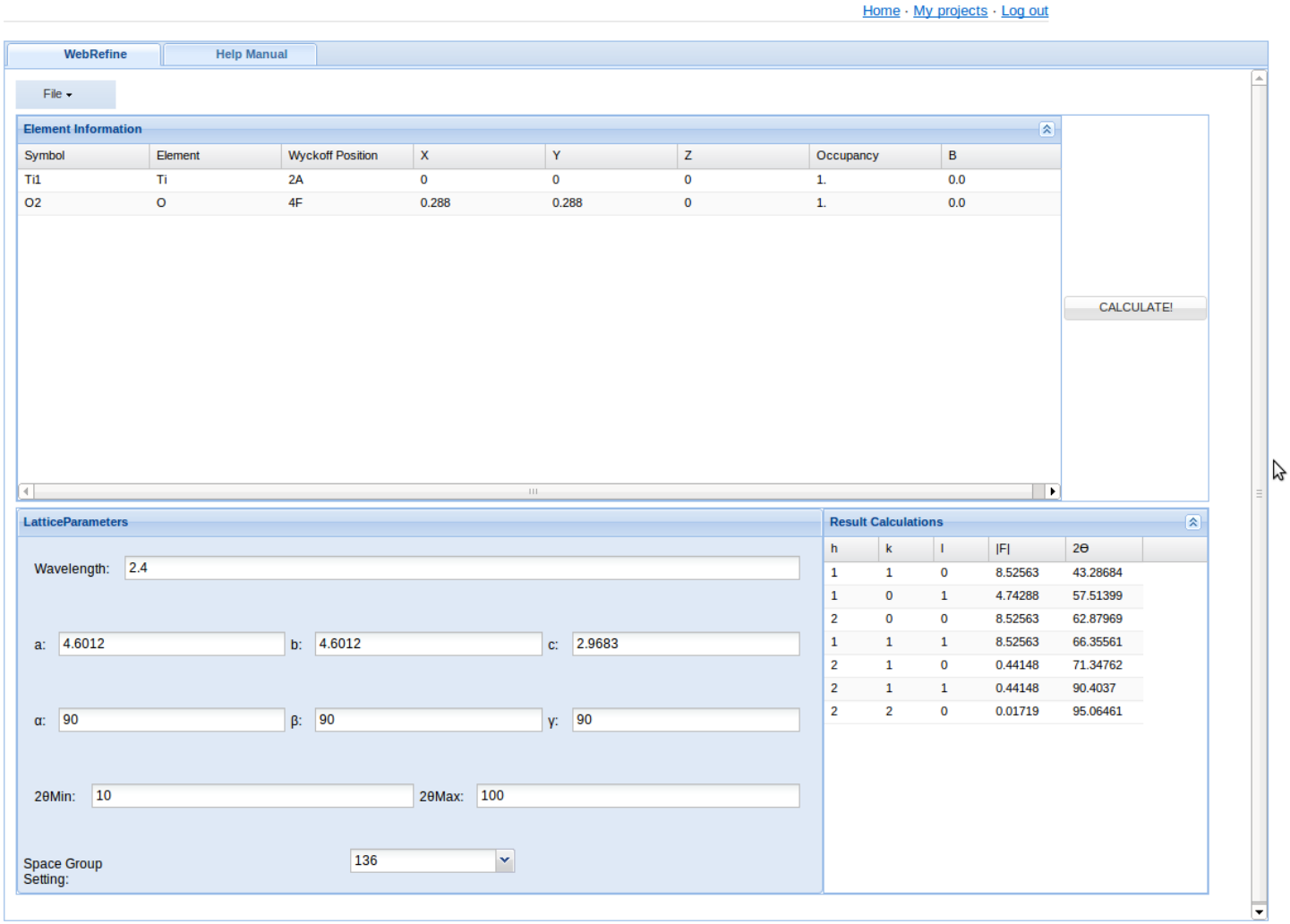



d
θ
dsinθ


(1 2 0)
(0 -2 2)
(-1 -1 1)
1/2
1/2
1/2
c
b
a
1/2
1/2
1/2
(1 1 2)
(2 0 1)
(0 0 2)

WebRefine

- Priyanka Patel (Poolesville)



Visitors

	Total	Unique	% Returning Visitor	Avg. Time on Site	Avg. Pages/Visit
Registered	2	1	50%	0:59:40	12
Guests	36	2	94.4%	0:00:31	1.2
Total	38	3	92.1%	0:03:38	3.9

Registered Users

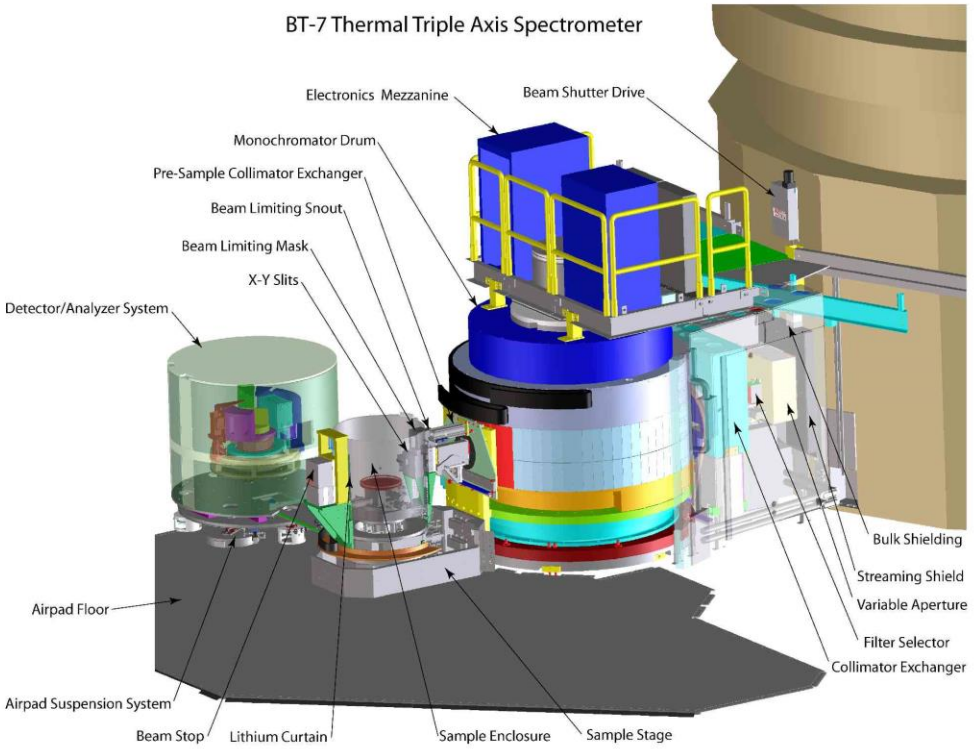
	# Visits	Avg. Time on Site	Avg. Pages/Visit
alexander	2	0:59:40	12

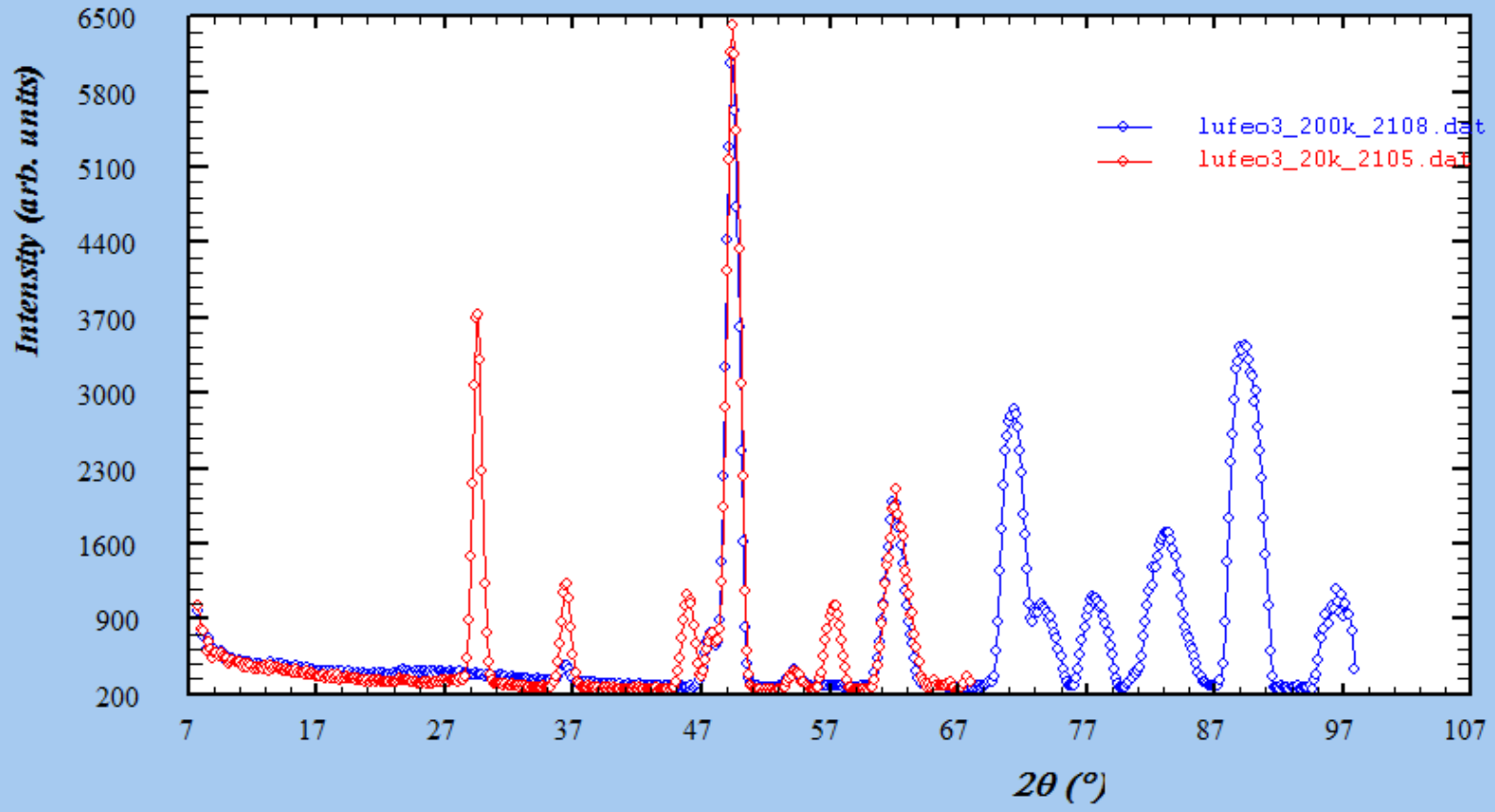
Pageviews

	Total	Unique
Registered	24	7
Guests	7	7
Total	31	14

Tracking began on Aug 05, 2013 @ 8:45:14 a.m.

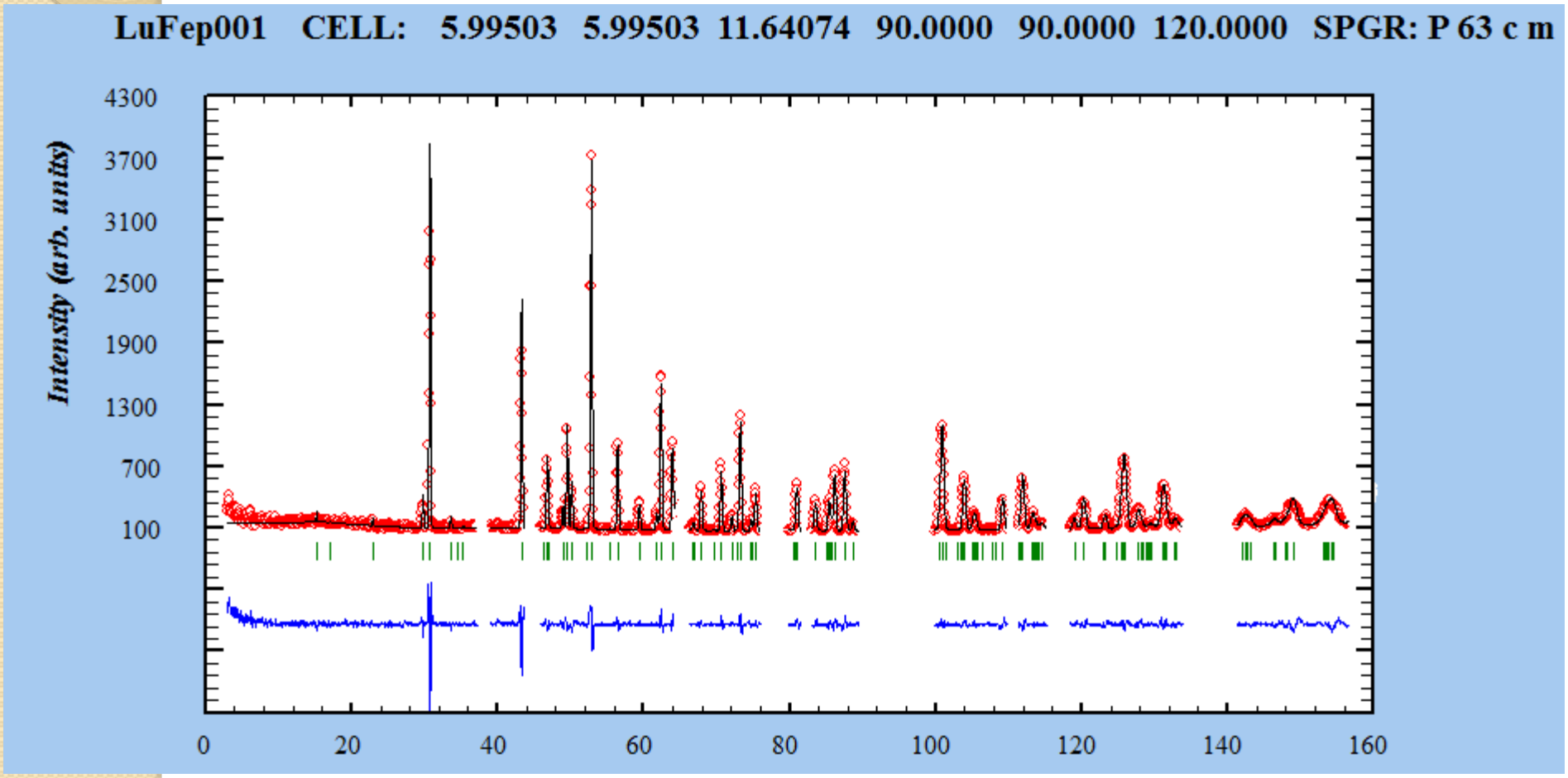
BT-1, BT-7, the Data Collectors




Intensity (arb. units)
6500
5800
5100
4400
3700
3000
2300
1600
900
200
7
17
27
37
47
57
67
77
87
97
107
2θ (°)
lufeo3_200k_2108.dat
lufeo3_20k_2105.dat

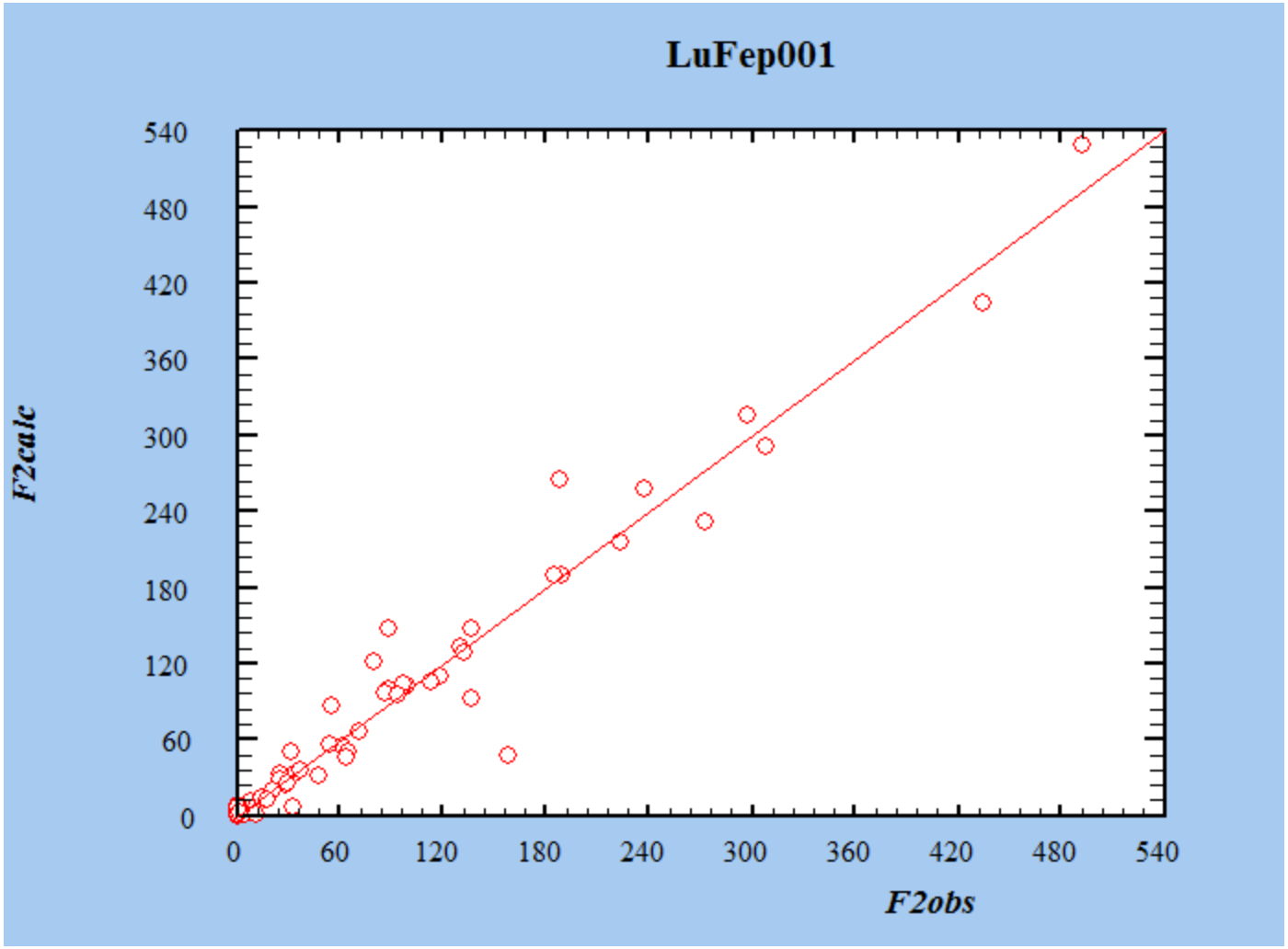
Fullprof

- Profile Refinement



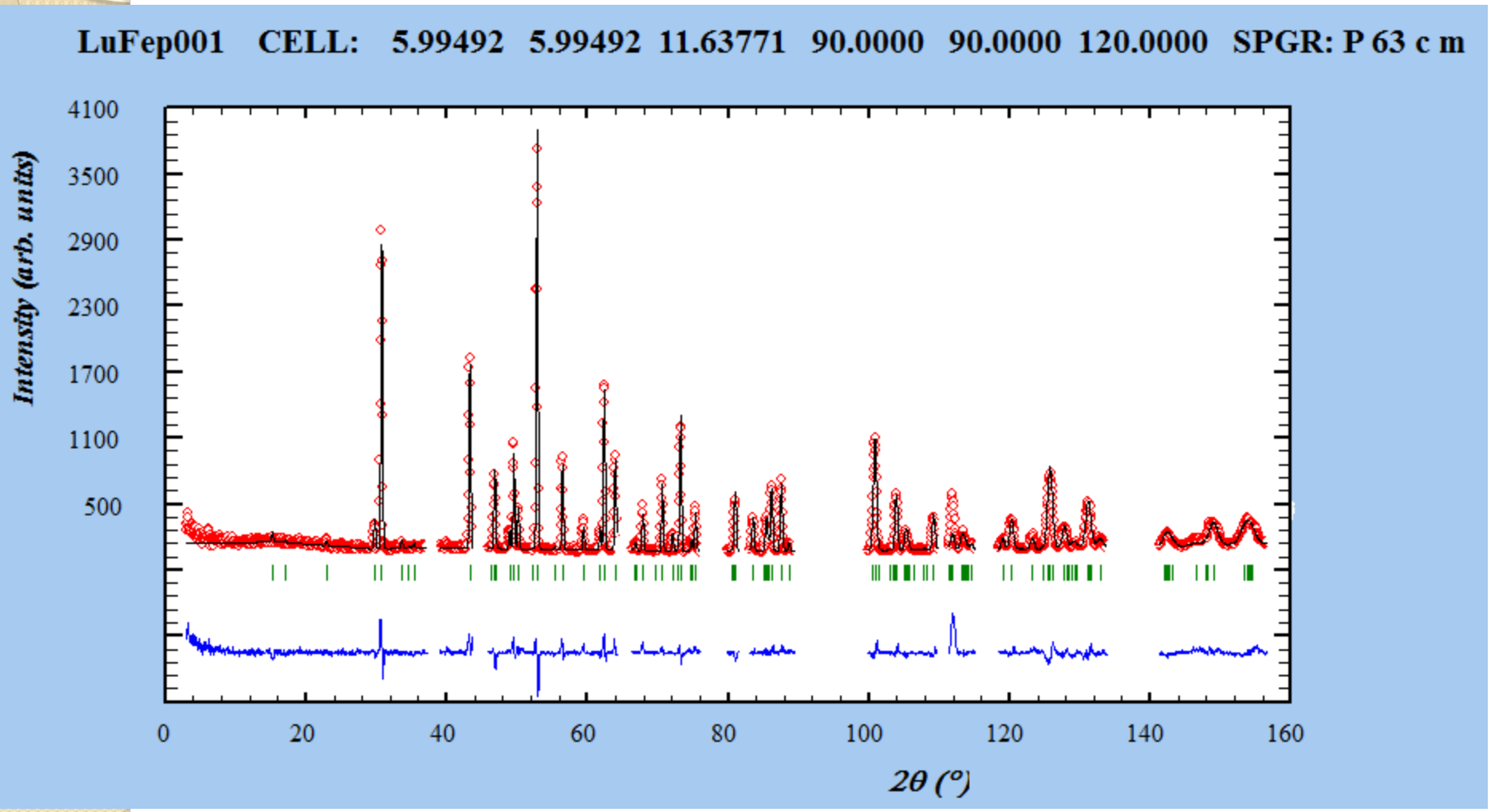
Fullprof (cont)

- Simulated Annealing



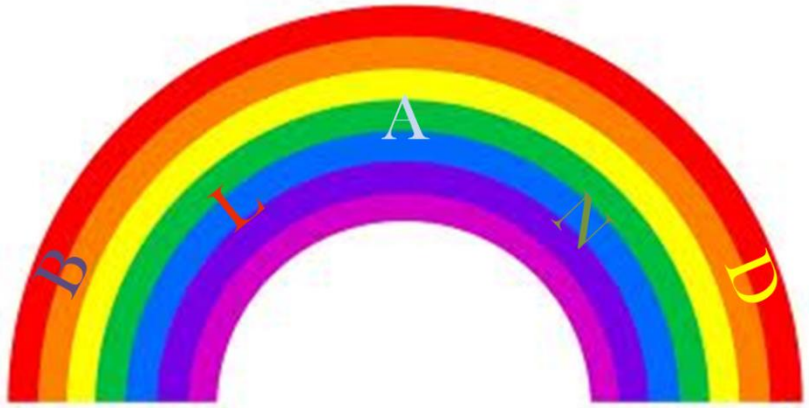
Fullprof (cont)

- Refinement

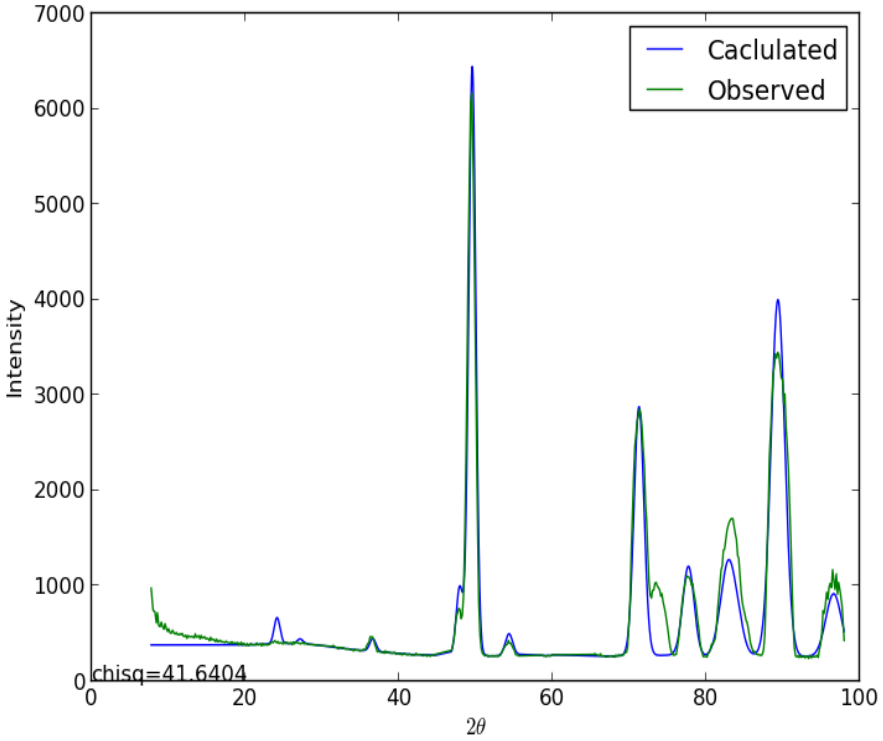


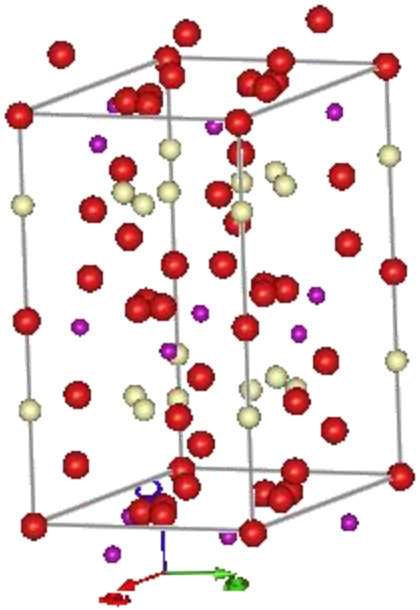
BLAND

- Goes through a range of values for each parameter to find the parameter that minimizes chi-squared value

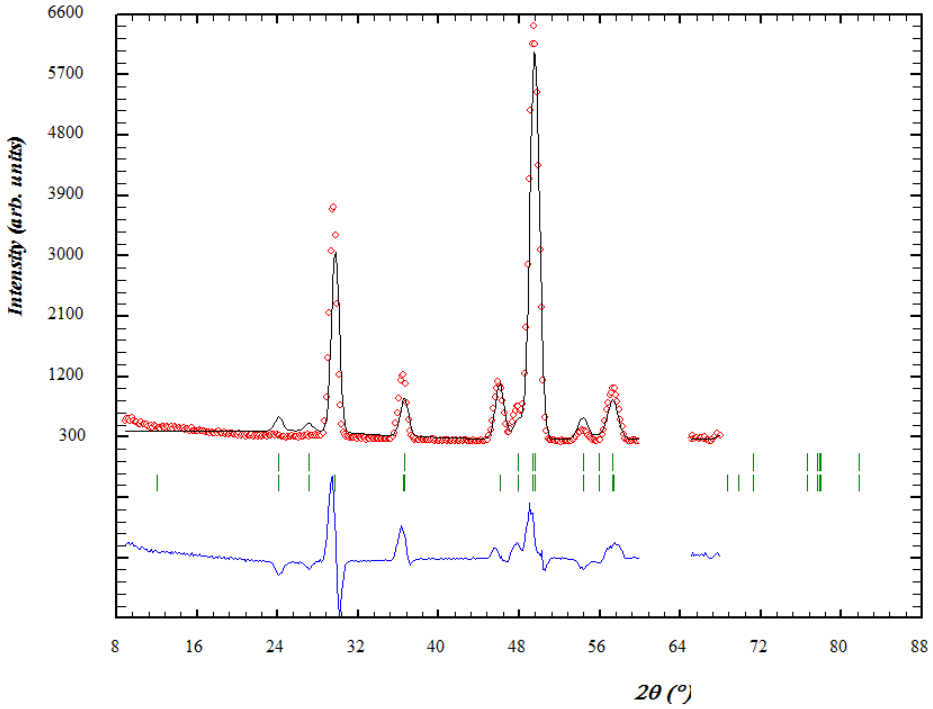


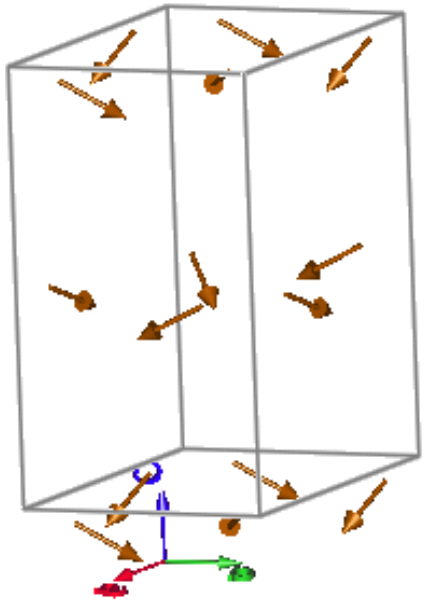
BLAND


Caclulated
Observed
Intensity
chisq=41.6404
2θ
0
1000
2000
3000
4000
5000
6000
7000
0
20
40
60
80
100

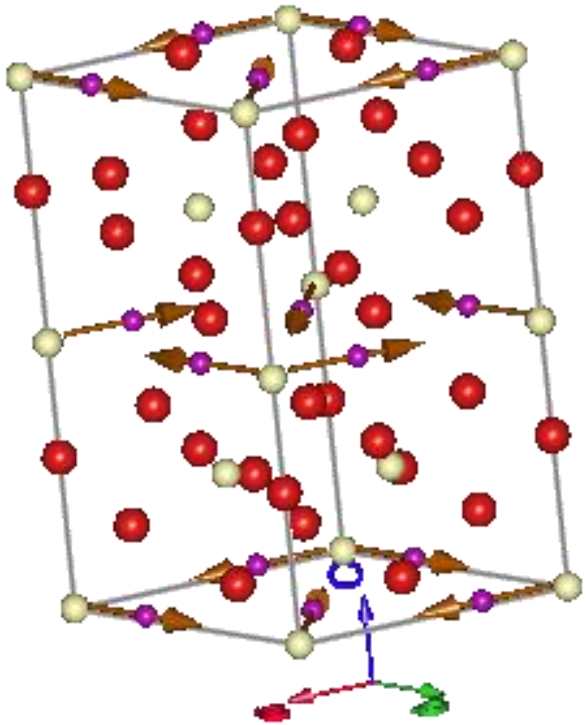


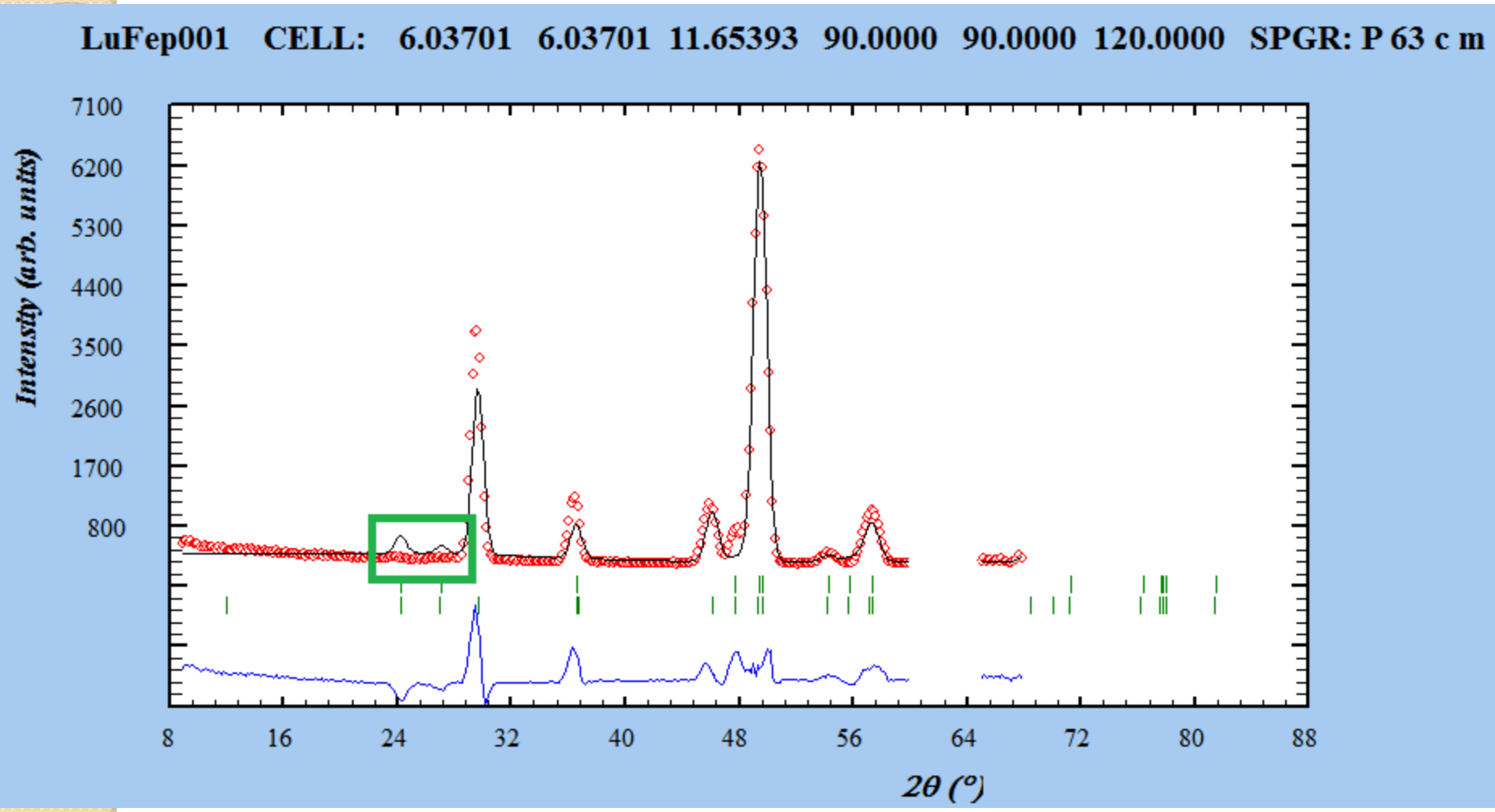
LuFep001 CELL: 6.02112 6.02112 11.70020 90.0000 90.0000 120.0000 SPGR: P 63 c m





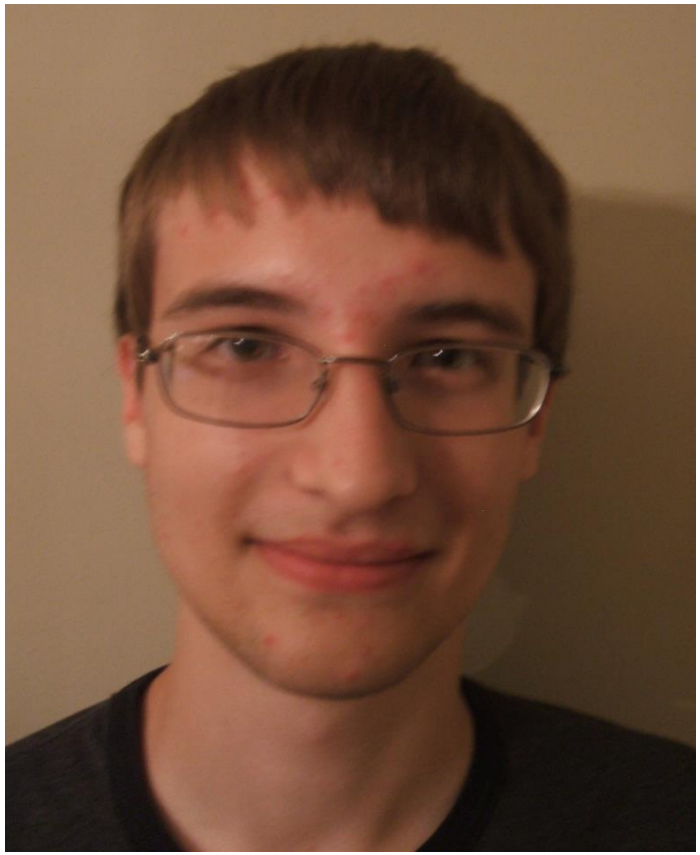
Most Updated Crystal/Magnetic Struc.




LuFep001 CELL: 6.03701 6.03701 11.65393 90.0000 90.0000 120.0000 SPGR: P 63 c m
Intensity (arb. units)
7100
6200
5300
4400
3500
2600
1700
800
8
16
24
32
40
48
56
64
72
80
88
2θ (°)

Acknowledgments

- Dr. William Ratcliff, my mentor
- Center for High Resolution Neutron Scattering (CHRNS), sponsor of NCNR SHIP
- Dr. Julie Borchers, Dr. Yamali Hernandez, coordinators of NCNR SHIP



- Dylan Quintana, the *bland* programmer

Sources

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- Martin, L. W., & Schlom, D. G. (2012). Advanced synthesis techniques and routes to new single-phase multiferroics. *Current Opinion in Solid State and Materials Science*, *16*(5), 199-215.
- "…I37 and the Hall hEIL Effect" | Reconciliation of Science and Religion. (n.d.). *Reconciliation of Science and Religion | Myth, math, and music, represent the scientific language of the ancients. This blog is an attempt to interpret those symbols left for us to observe.*. Retrieved August 7, 2013, from http://kachina2012.wordpress.com/2011/11/09/i37-and-the-hall-heil-effect/