Iron-based Magnetic Superconductors

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Outline

- (Brief) History of Magnetic Superconductors
  - Magnetic Impurities
  - Long Range Magnetic Order: Coexistence and Competition
- Cuprate Superconductors—Highly Correlated Electron Systems
  - Undoped systems: Mott Insulators. Magnetic Order and Spin Waves
  - Doping dependence of properties
- Magnetic Properties of Iron-based Superconductors
- Summary

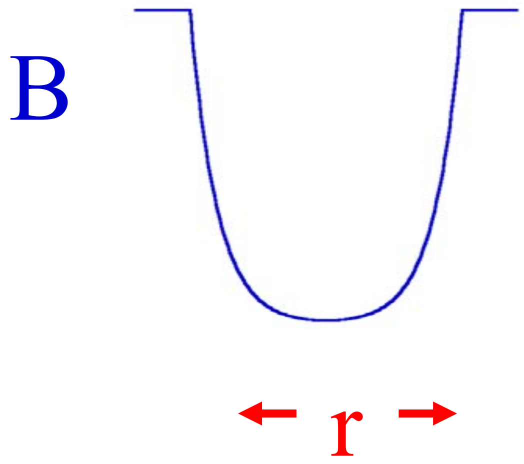
Super?conductivity

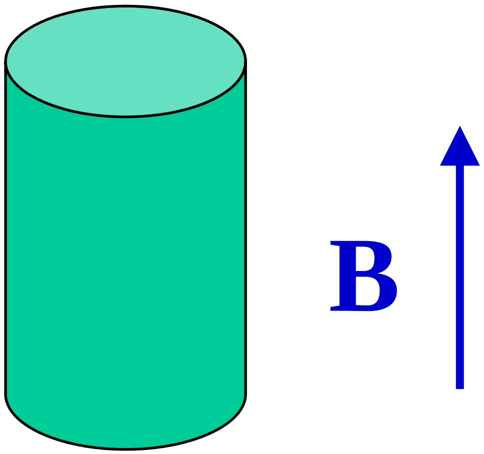
Perfect conductor   R=0   But currents decay

B first, then R=0; field will be maintained

Meissner Effect: Flux is expelled →***Superconductor !***

London Penetration Depth λ   ~500 Å





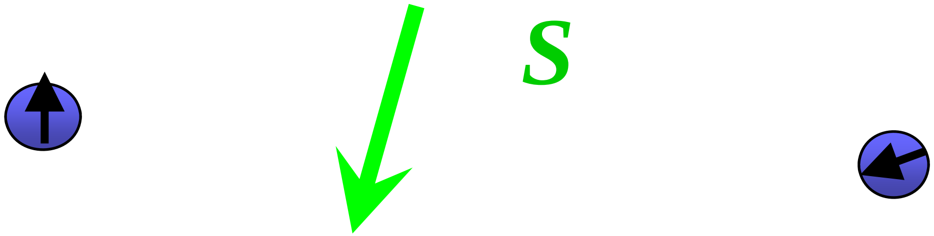
Superconducting Energetics

Cooper Pair (Energy gap Δ)

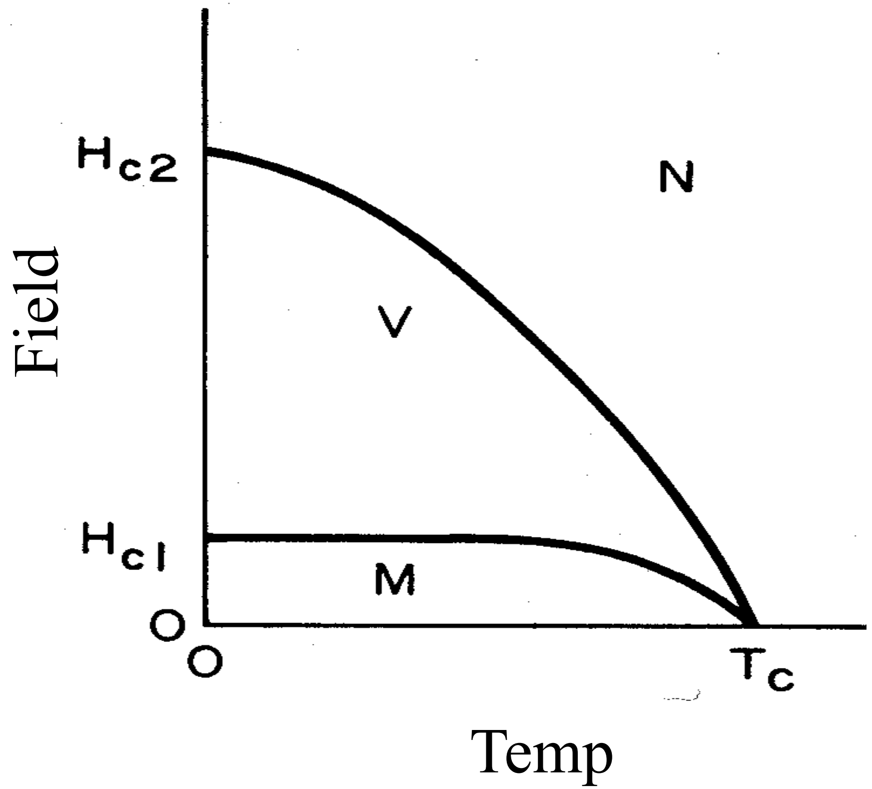
$(\boldsymbol{k}\uparrow; -\boldsymbol{k}\downarrow)$ $\Delta = 3.5\ kT_C$

Coherence Length ξ ~25 Å

Spin depairing (Anderson; Abrikosov-Gor'kov)

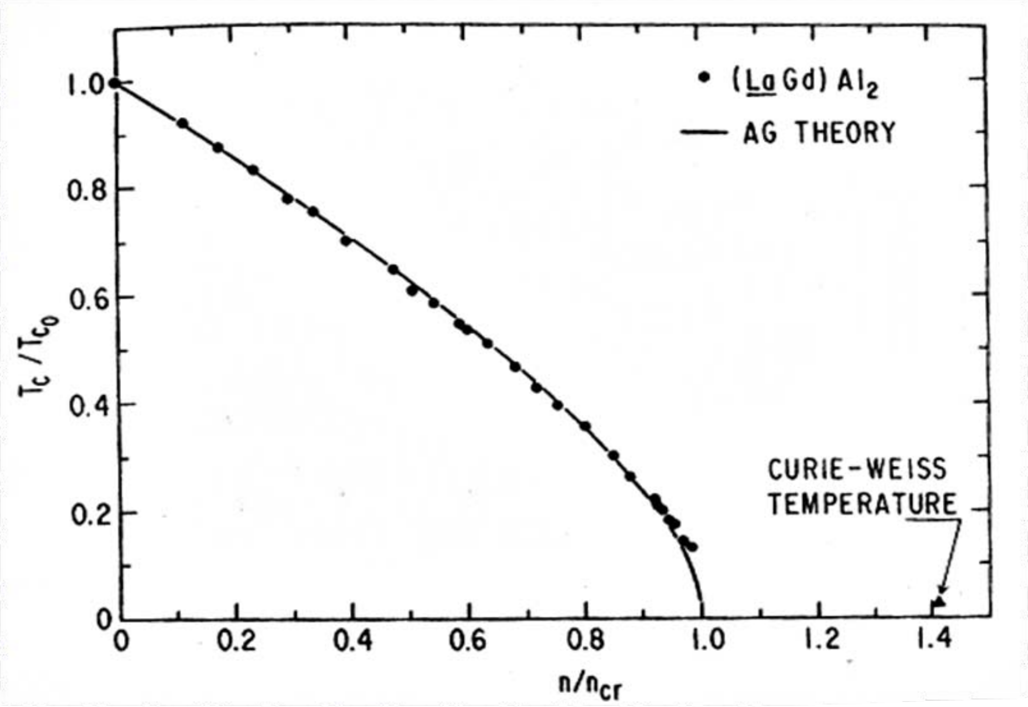


Magnetism and Superconductivity are Antagonists



Magnetic Impurities Cause Spin depairing

T_C



Magnetic Concentration

M. B. Maple, Appl. Phys. **9**,179 (1976)

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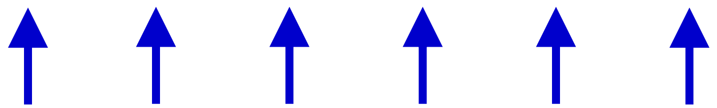
Magnetic Superconductor History

$$\left(k\uparrow; -k\downarrow\right)$$

- Pure Superconductors
- **X** Magnetic Impurities **X**
- Concentrated Magnetic Systems (Exceptions to the Rule!)
  - C-15 Cubic Laves phase (Ce-Ho)Ru_2 ('60's-'70's)
- Magnetic Sublattice—Long Range Order
  - Chevrel Phase $DyMo_6S_8$ ('70's)
- Ferromagnets—Competition & Coexistence
  – Chevrel Phase $HoMo_6(S\text{-}Se)_8$, $ErRh_4B_4$ ('70's – 80's)
- High T_C cuprates—Cu spin order & fluctuations
  - Cuprates $RBa_2Cu_3O_7$ [123], R_2CuO_4 [214] ('80's→…) ⇐
- Borocarbides
  – $HoNi_2B_2C$, $ErNi_2B_2C$ ('90's→…)
- New Ferromagnetic Superconductors
  – Ruthenates $RuSr_2GdCu_2O_8$, $RuSr_2(Eu\text{-}Ce)_2Cu_2O_{10}$; $ZrZn_2$, UGe_2 (2000's →…)
- Sodium cobaltates (Magnetic, thermoelectric, and Superconducting) 2000's→…
  – Na_xCoO_2 (+ H_20) [just add water for superconductivity !] ⇐
- Iron-based superconductors (Feb, 2008→…)
  – $R(O_{1-x}F_x)FeAs$; $Sr_{1-x}K_xFe_2As_2$; LiFeAs; $Fe(Se_{1-x}Te_x)$
  – 1:1:1:1 1:2:2 1:1:1 1:1

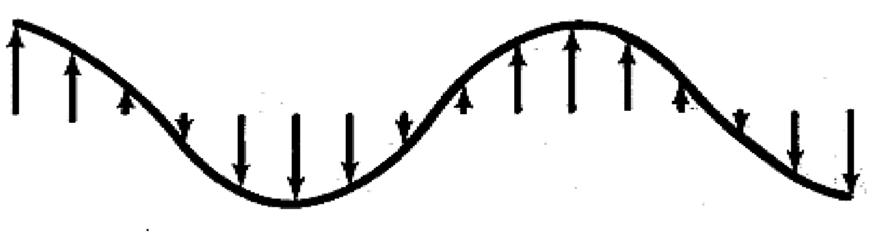
Magnetic Structures

Ferromagnet



Antiferromagnet

Spin Density Wave



Iron-based superconductors under Investigation at the NCNR

- $LaO_{1-x}F_xFeAs$ LaOFeAs (1:1:1:1)
- $CeO_{1-x}F_xFeAs$ CeOFeAs
- $NdO_{1-x}F_xFeAs$ Nd…
- $PrO_{1-x}F_xFeAs$ Pr…
- $BaFe_2As_2$, $SrFe_2As_2$, $CaFe_2As_2$ (1:2:2)
- $CaFe_2As_2$, Under Pressure
- Fe_{1+x}(Se-Te) (1:1)
- LiFeAs (1:1:1)
  - http://www/ncnr.nist.gov/staff/jeff

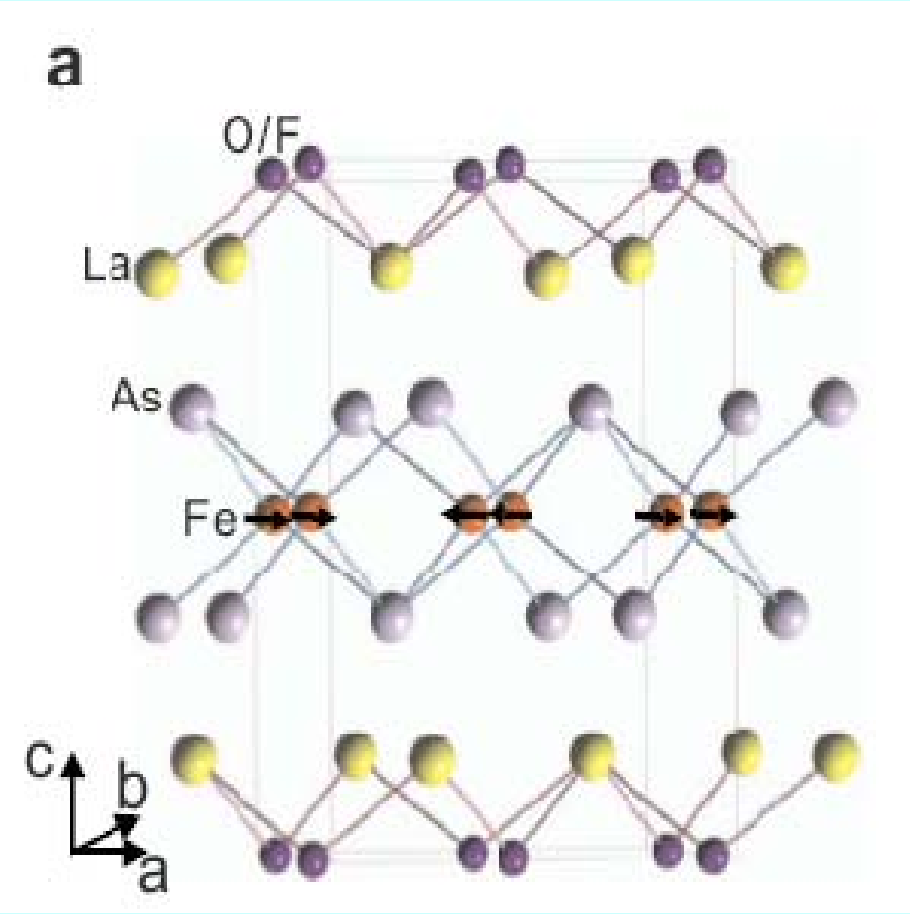
Collaborations

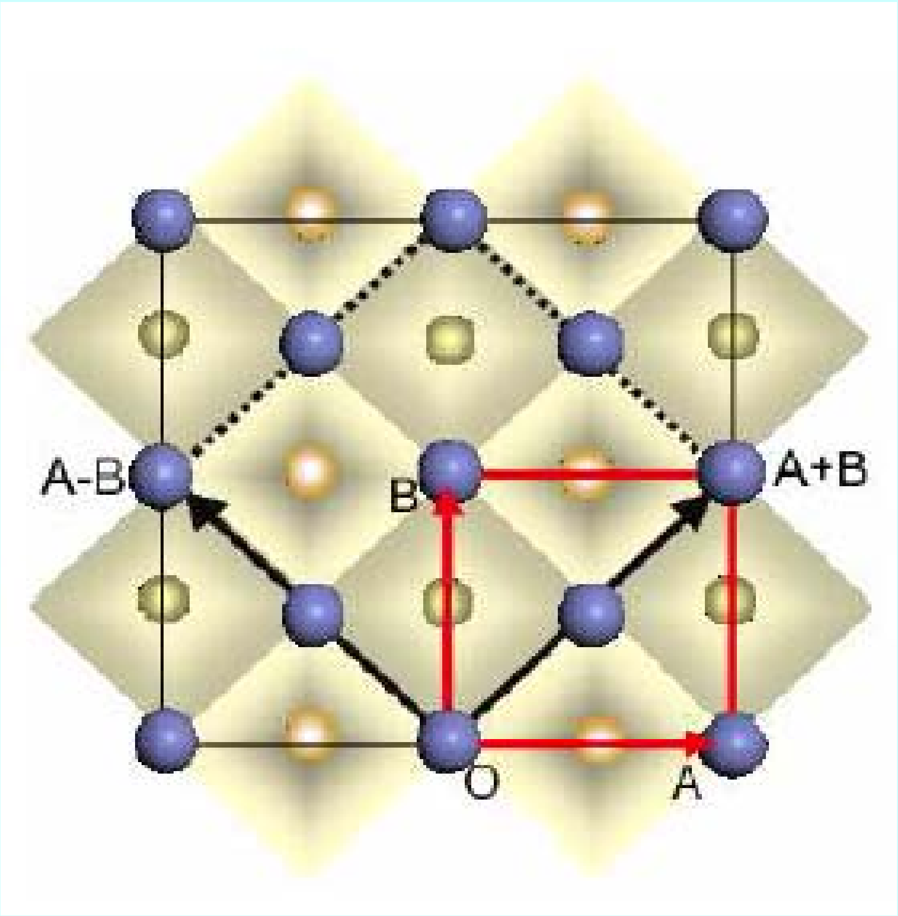
- U. Tennessee/ORNL (Pengcheng Dai, et al.)
  - Beijing Institute of Physics (Nan Ling Wang, et al.)
- LANL (Wei Bao, et al.)
  - USTC (Xian-Hui Chen, et al.)
- Princeton University (Bob Cava, et al.)
- Iowa State University/Ames Lab (Alan Goldman, Andreas Kreyssig, Paul Canfield, Rob McQueeney, et al.)
- Tata Institute of Fundamental Research (Sudesh Dhar)
- University of Maryland (Johnpierre Paglione)
- NCNR (Qing Huang, William Ratcliff, Ying Chen, Sung Chang, Ben Ueland, Pawel Zajdel, Mark Green, Yiming Qiu, Craig Brown, Taner Yildirim, John Copley, Jasmine Millican, Daniel Phelan, Juselino Leao, Sarah Poulton)

Properties of *RE*(O,F)Fe(As,P)

- Parent Materials
  - Metallic (poor metal)
  - Anisotropic (ranging from 5 – 30)
  - Have a structural distortion (T ~ 150 K)
  - Fe spins are antiferromagnetically ordered (T_N ~ 140 K)
- Superconductors
  - T_C as high as 55 K
  - Anisotropic (but not nearly as much as the cuprates)
  - Very high upper critical fields (60 T)

Crystal Structure of La(O,F)FeAs





Magnetic Order Close to Superconductivity in the Iron-based Layered La($O_{1-x}F_x$)FeAs systems, C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. Dai,
Nature **453**, 899 (2008).

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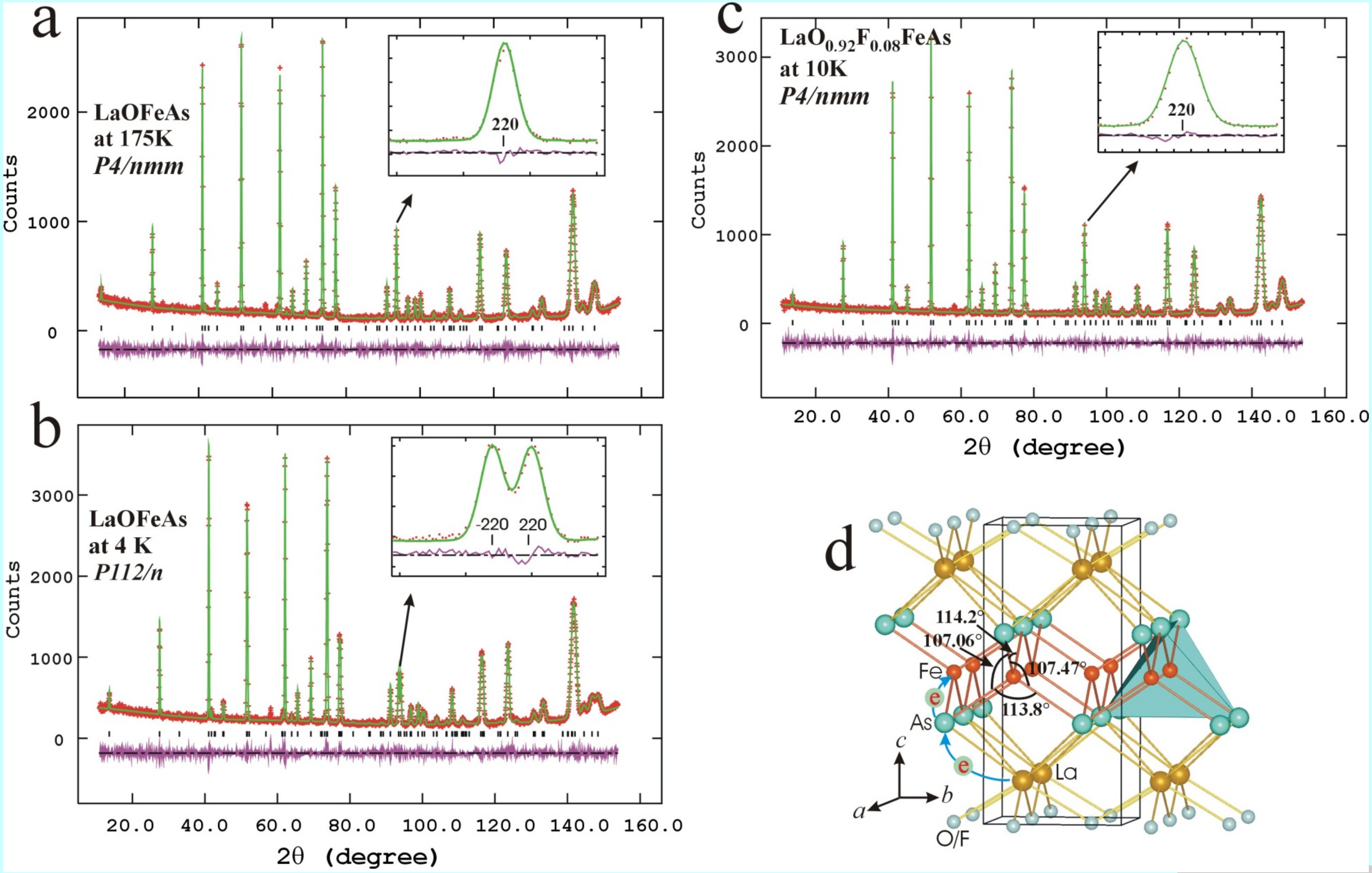
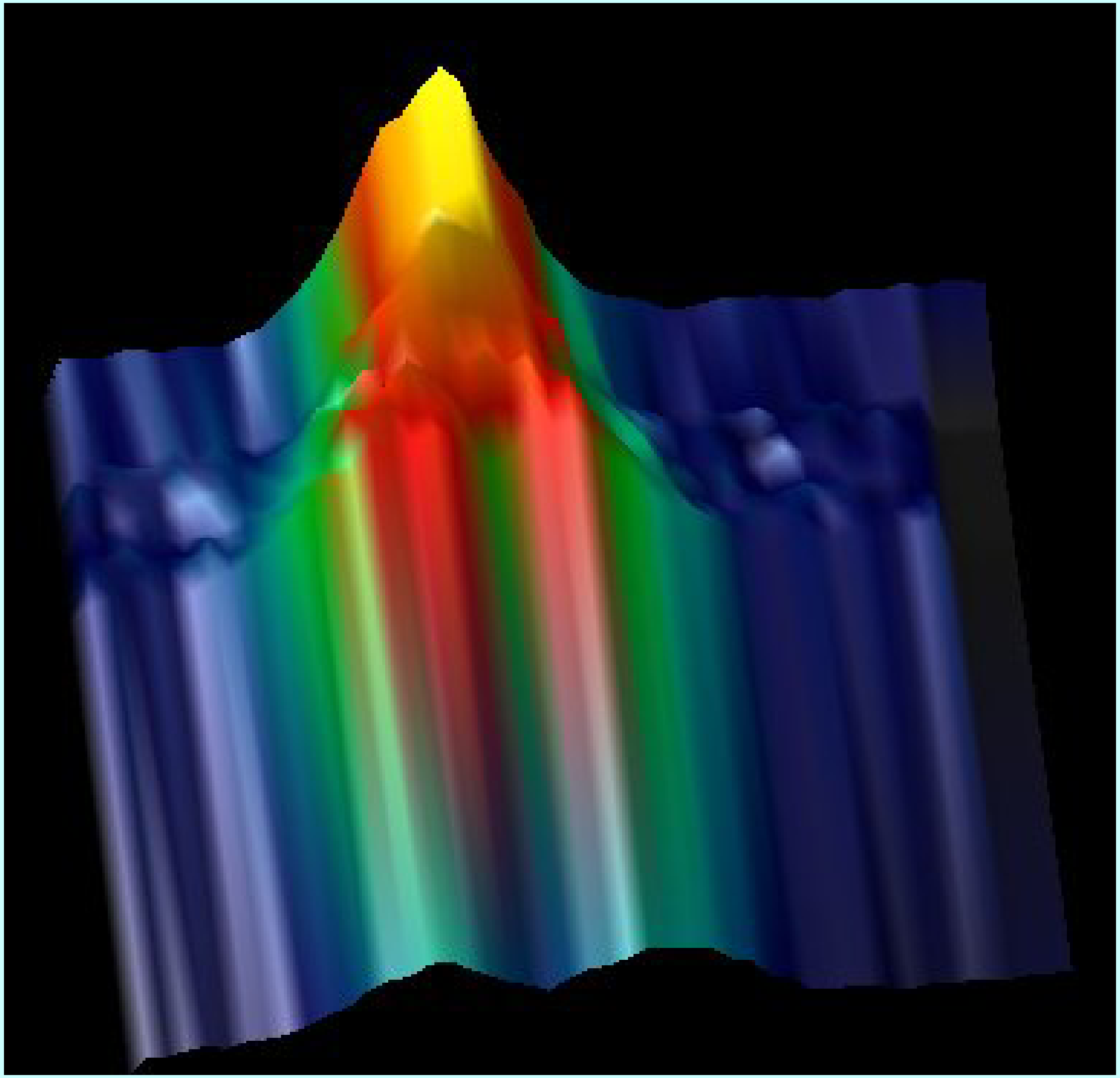
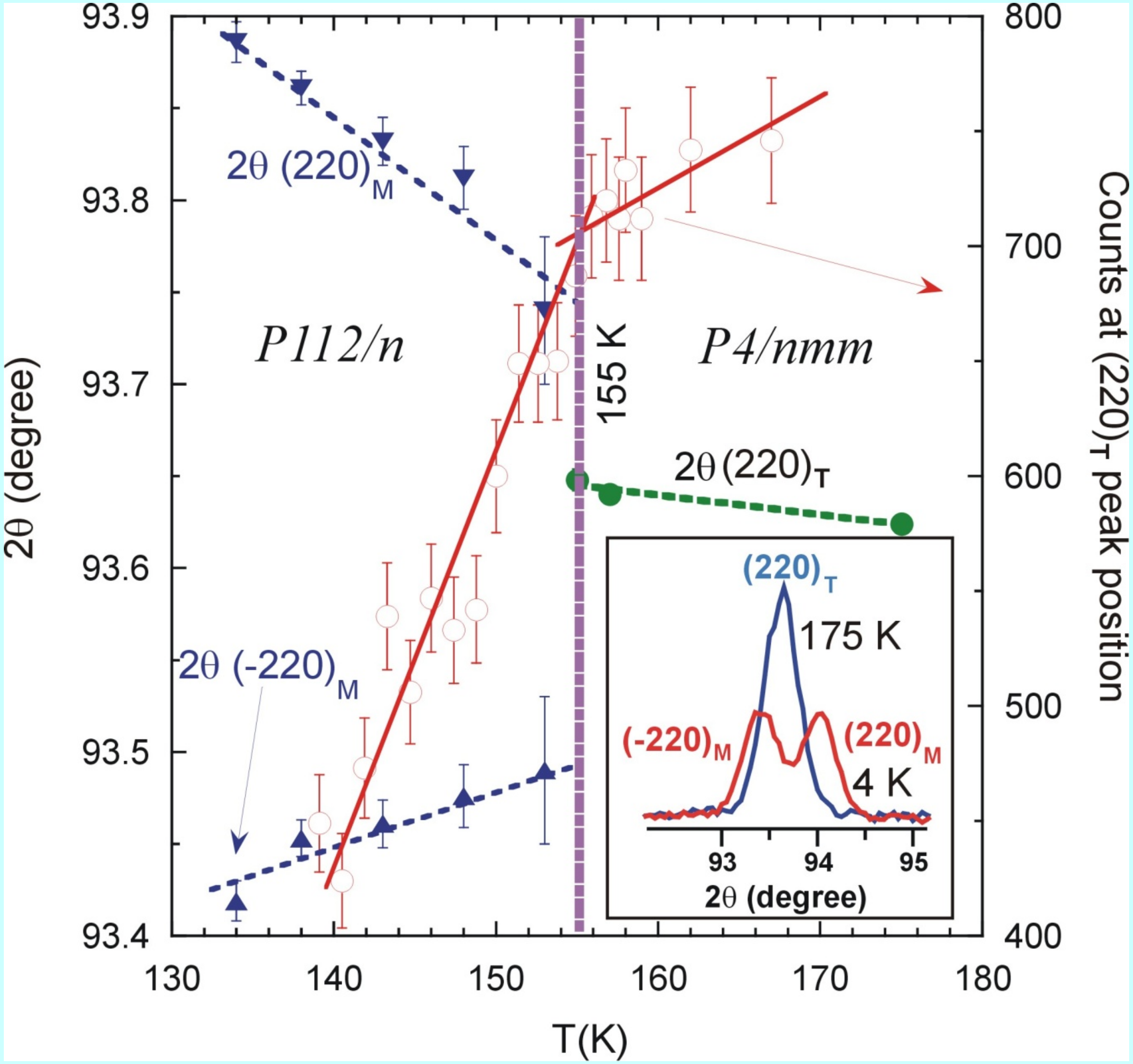
Crystal Structure of La(O,F)FeAs



Crystal Structure of La(O,F)FeAs

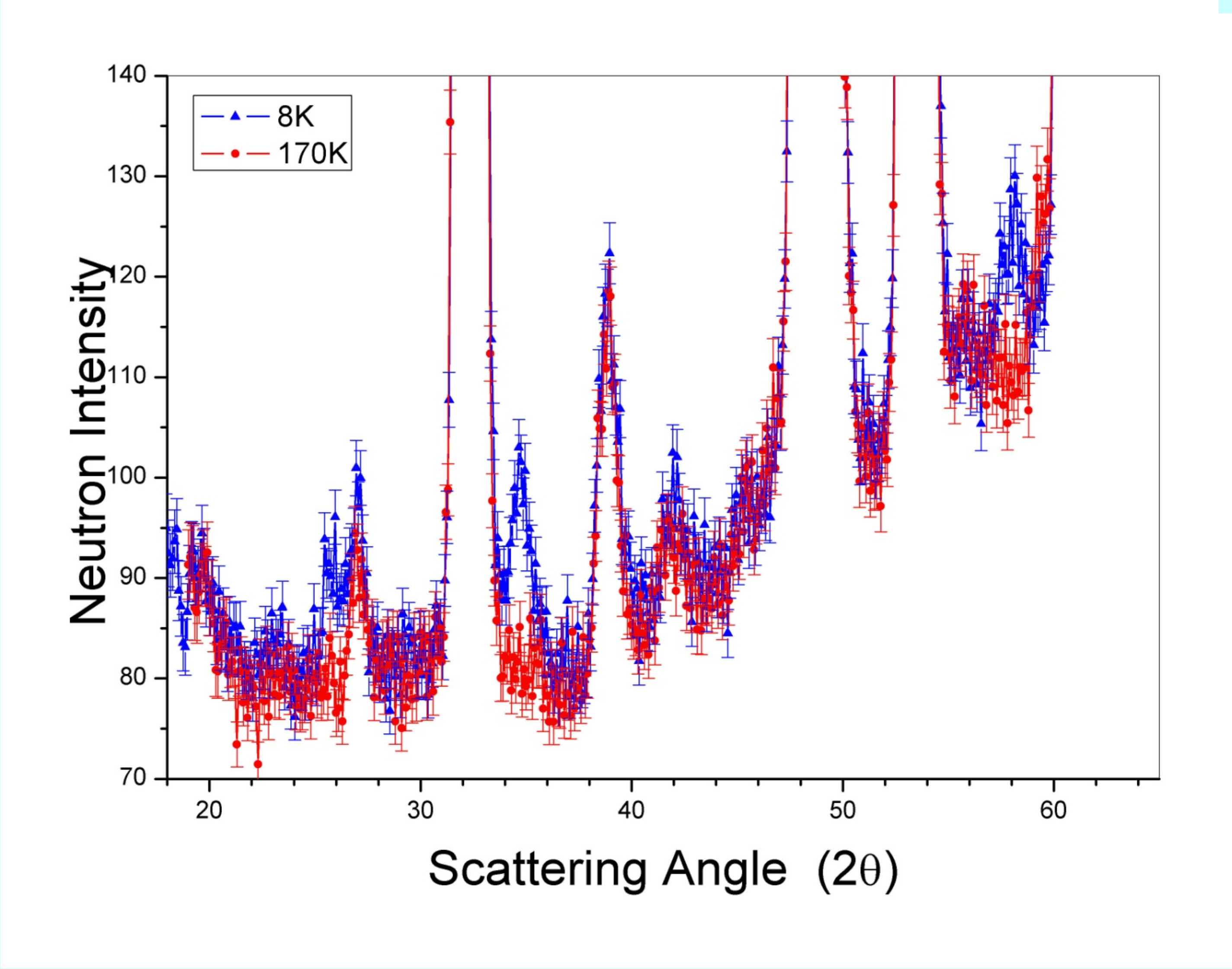


Crystal Structure of La(O,F)FeAs

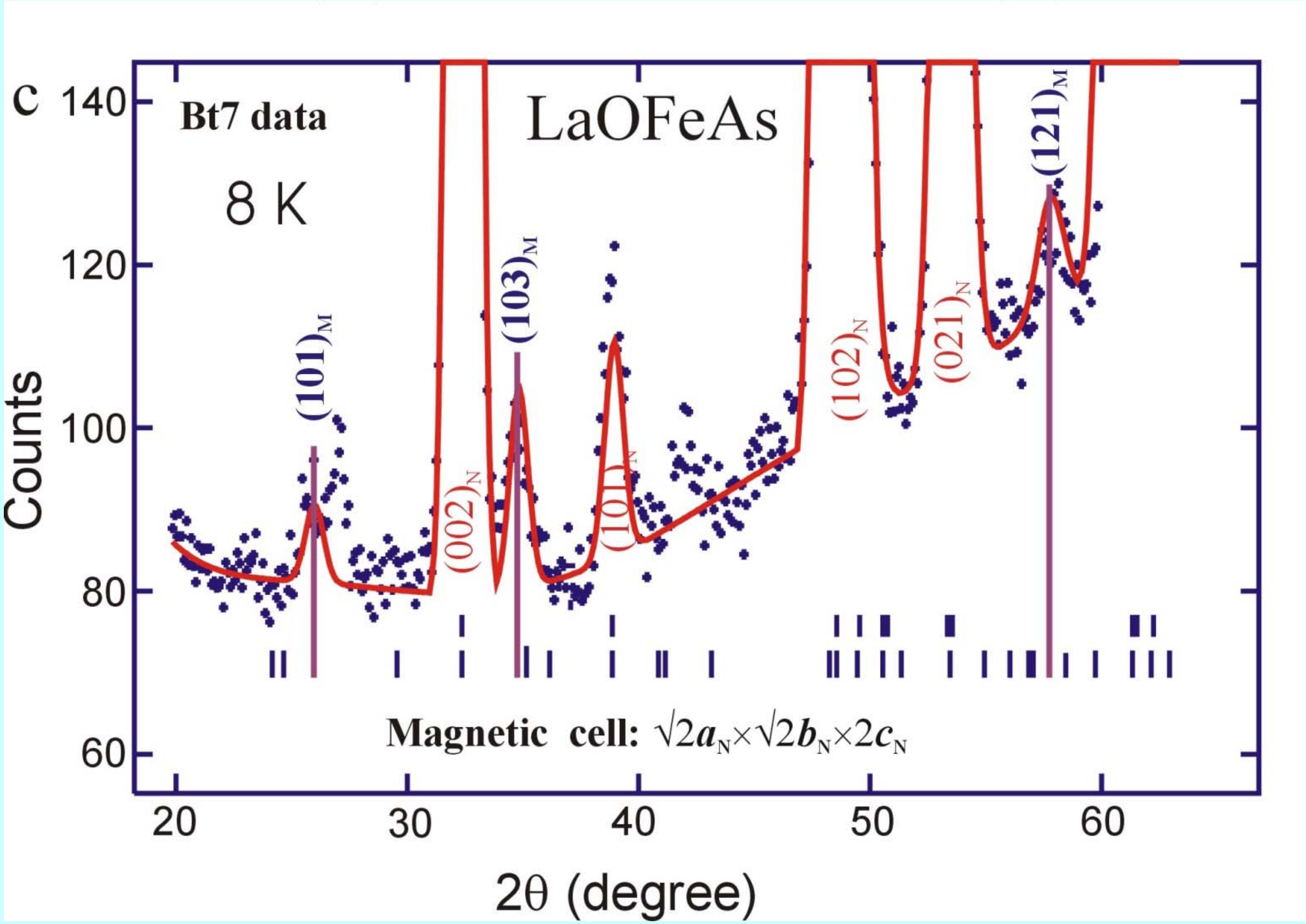


Magnetic Scattering from La(O,F)FeAs

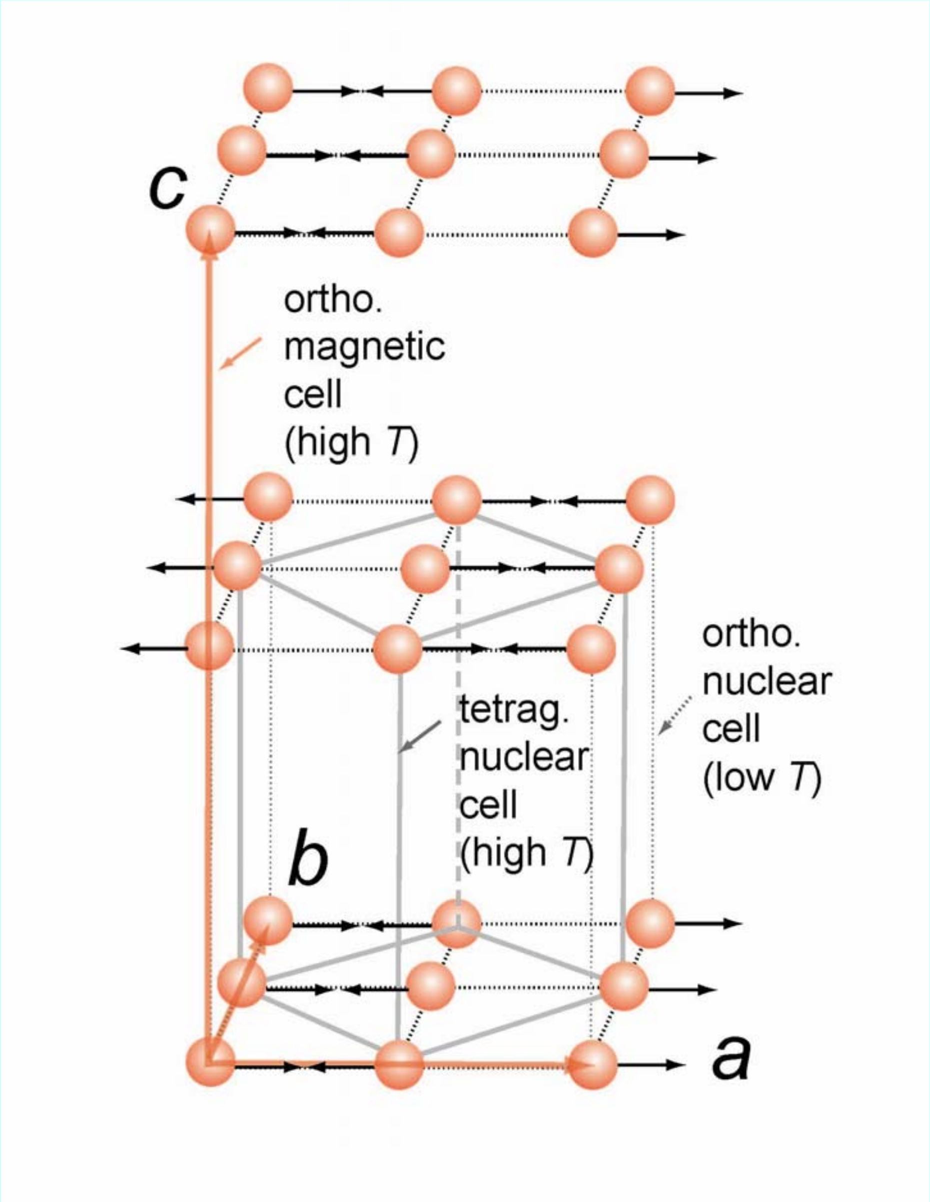
PSD on BT-7



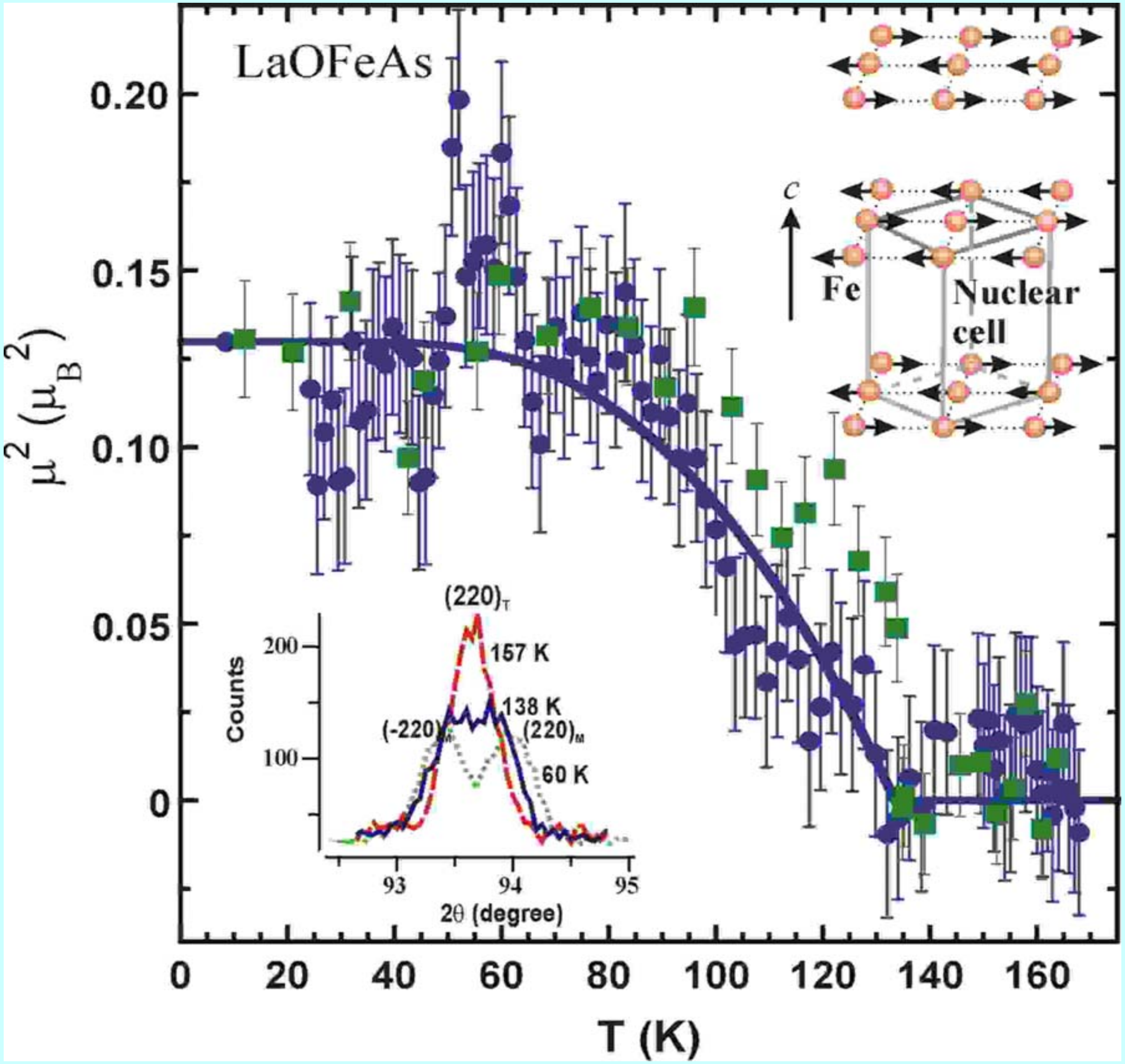
Magnetic Structure La(O,F)FeAs



Magnetic Structure of La(O,F)FeAs



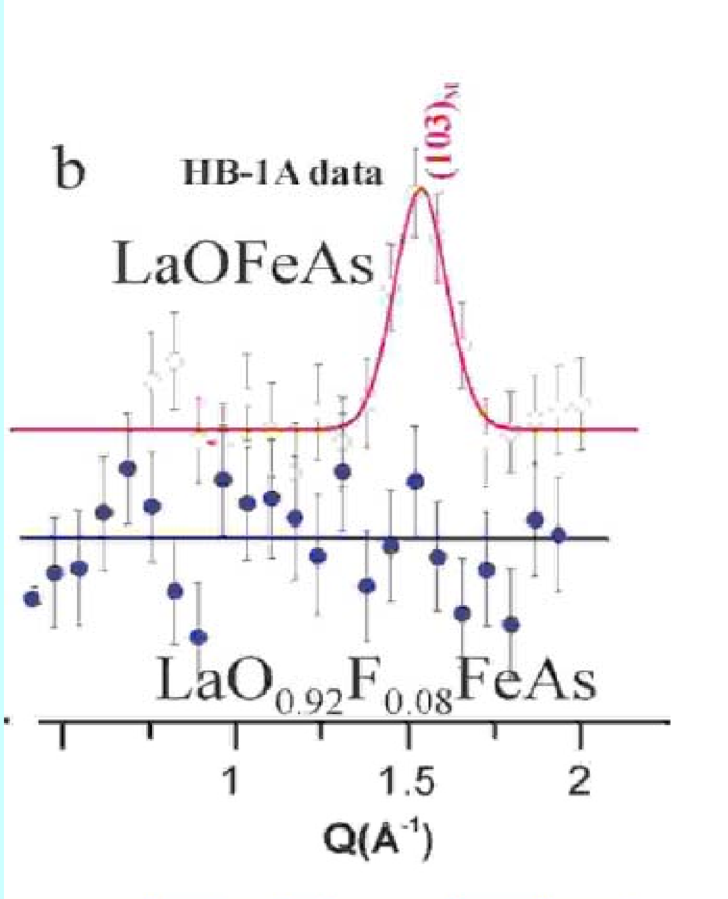
Magnetic Structure LaOFeAs



Is it a Spin Density Wave?

- It's metallic
- *d*-bands are at the Fermi Surface (like Fe, Ni, Cr)
- Local moment—bands should be fully split
- Small moment (typically $<1\ \mu_B$)
- Spin Dynamics are energetic
  - (band energies (~0.2 eV) rather than kT_N)
- But the magnetic structure is commensurate

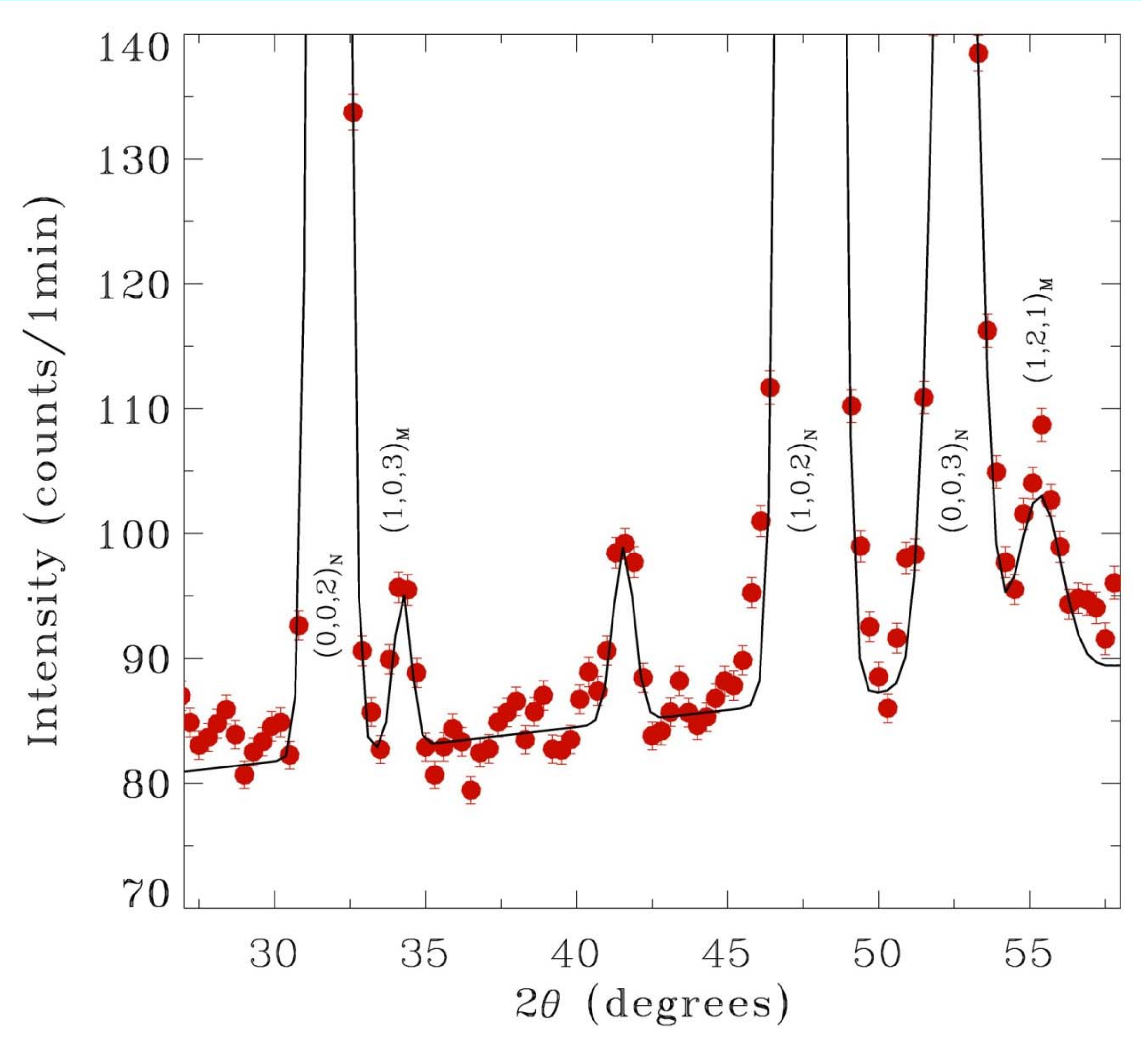
Comparison of Parent and Superconducting La(O,F)FeAs



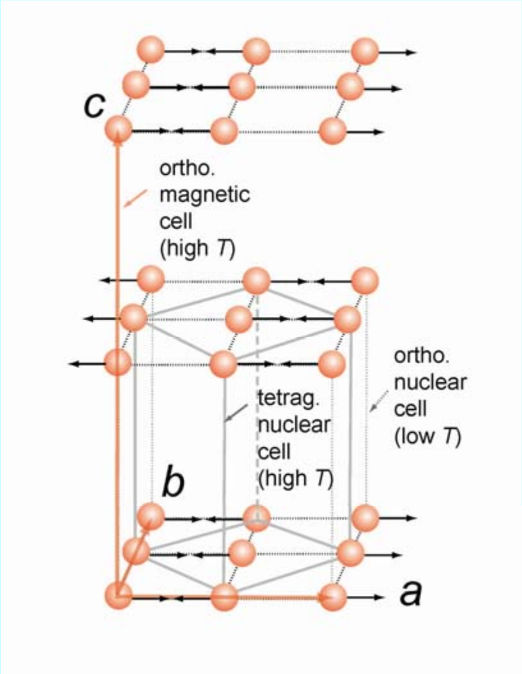
Properties of *Nd*(O,F)FeAs
T_C = 52 K

- Magnetic Order of the Iron Spins in NdOFeAs, Y. Chen, J. W. Lynn, G. F. Chen, G. Li, Z. C. Li, J. L. Luo, N. L. Wang, P. Dai, C. dela Cruz, and H. A. Mook, Phys. Rev. B**78,** 064515 (2008).
- Structure and Magnetic Order in the $NdFeAsO_{1-x}F_x$ Superconductor System, Y. Qiu, W. Bao, Q. Huang, T. Yildirim, J. M. Simmons, M. A. Green, J.W. Lynn, Y.C. Gasparovic, J. Li, T. Wu, G. Wu, and X.H. Chen, Phys. Rev. Lett. **101**, 257002 (2008).

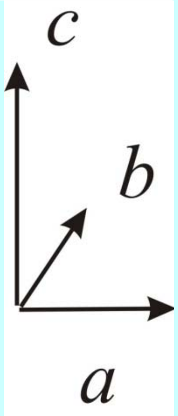
NdOFeAs



Intensity (counts/1min)
140
130
120
110
100
90
80
70
30
35
40
45
50
55
2θ (degrees)
(0,0,2)N
(1,0,3)M
(1,0,2)N
(0,0,3)N
(1,2,1)M

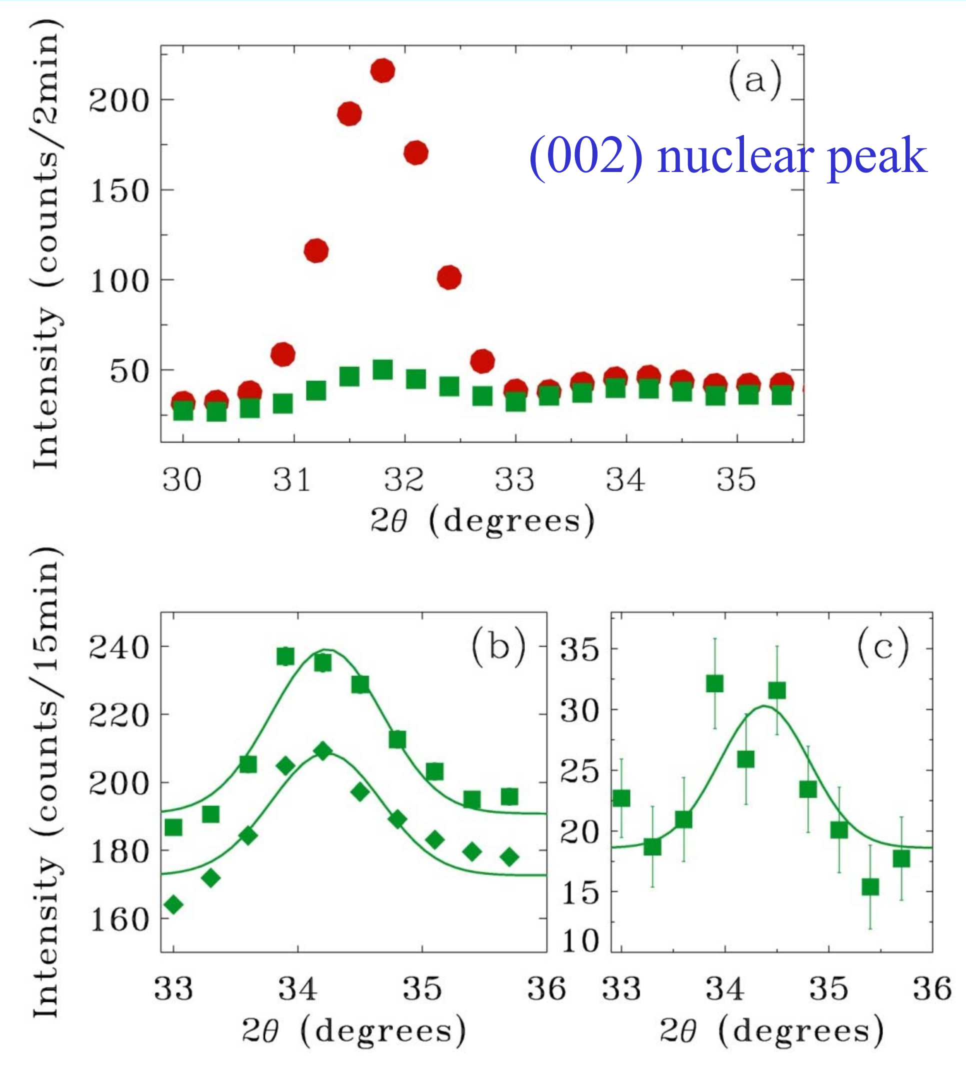


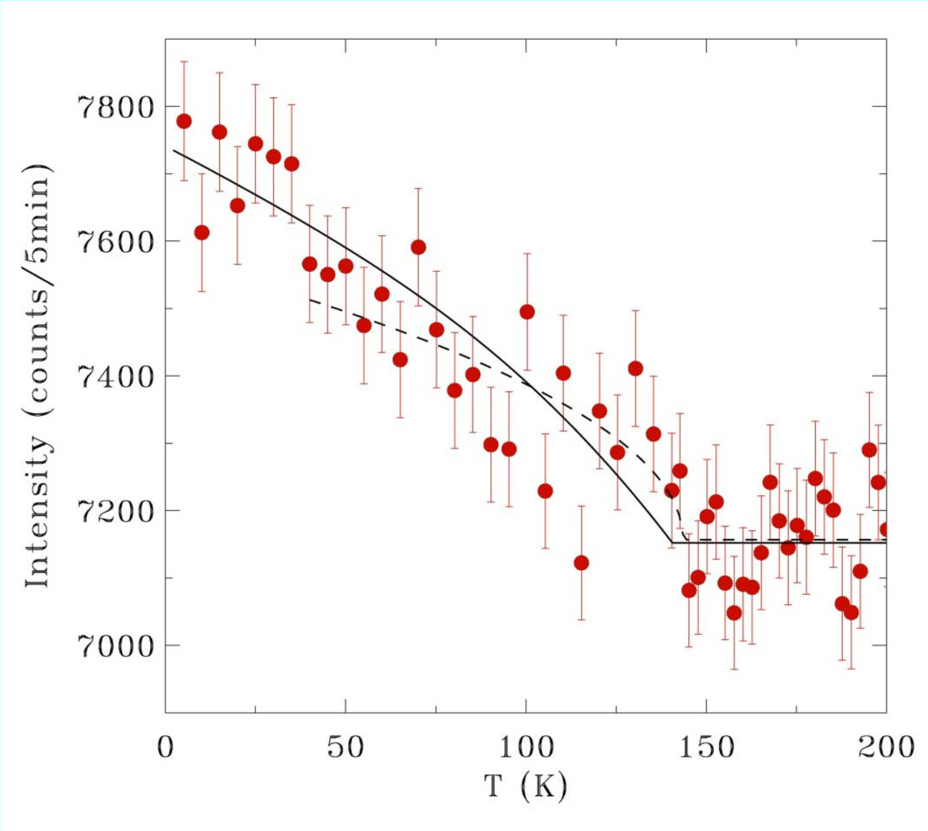
c
ortho.
magnetic
cell
(high T)
b
tetrag.
nuclear
cell
(high T)
ortho.
nuclear
cell
(low T)
a



c
b
a

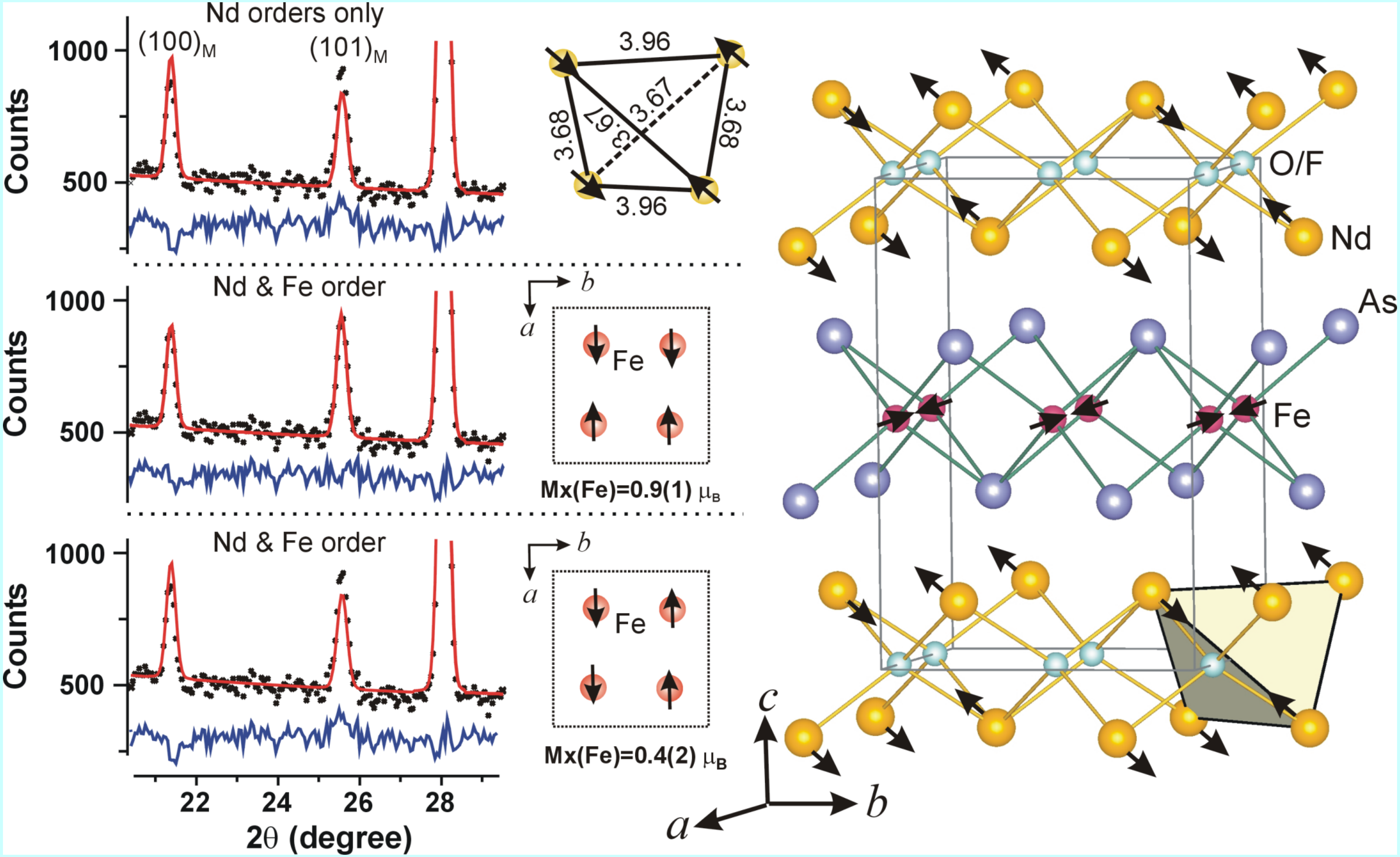
NdOFeAs





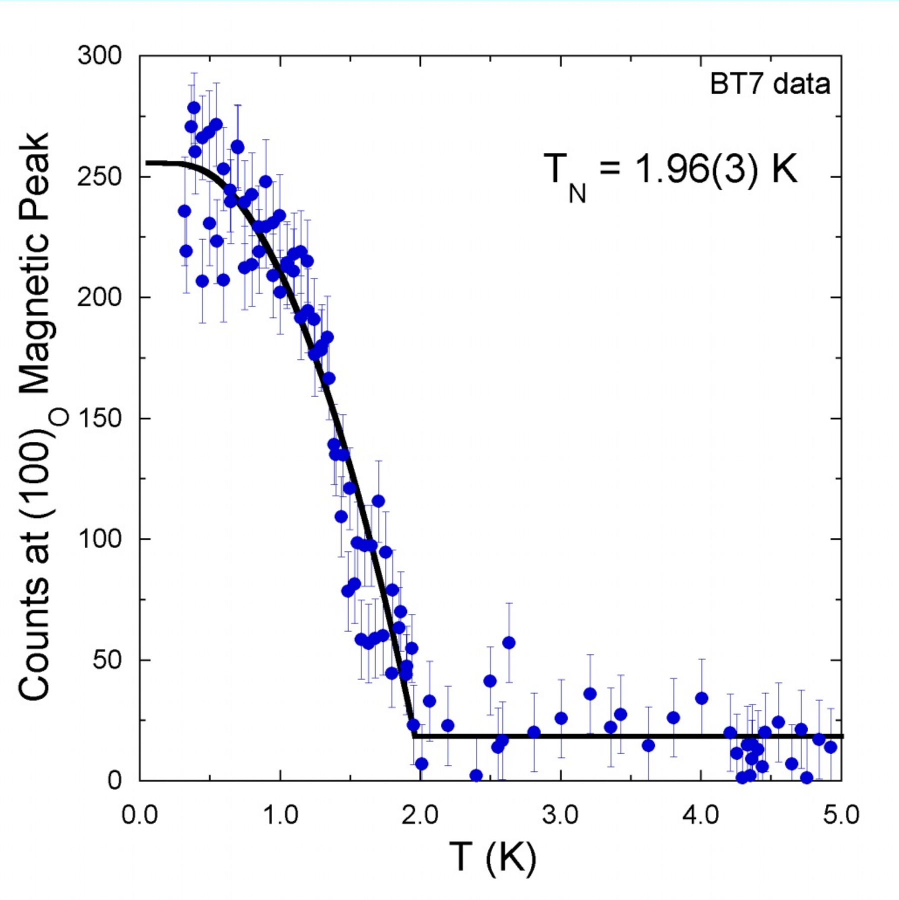
Polarized Beam (**P**||**Q** (squares) and **P**⊥**Q** (diamonds))

NdOFeAs

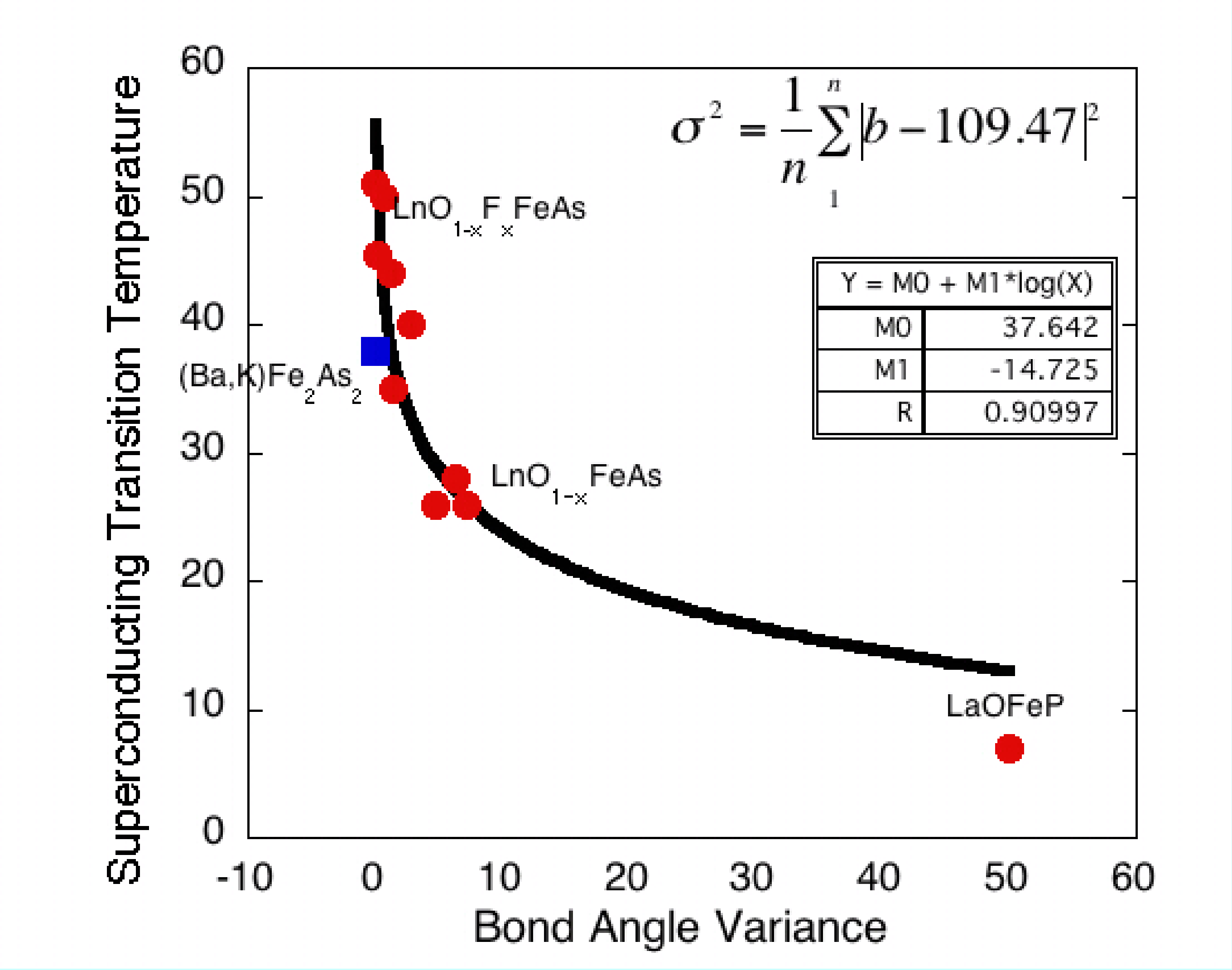


Nd orders only
(100)M
(101)M
Counts
1000
500
3.96
3.67
3.67
3.68
3.68
3.96
Nd & Fe order
b
a
Fe
Mx(Fe)=0.9(1) μB
Nd & Fe order
Fe
Mx(Fe)=0.4(2) μB
22
24
26
28
2θ (degree)
O/F
Nd
As
Fe
c
b
a

NdOFeAs Structure



Tc—Structure Relationship



Doping Dependence of La(O,F)FeAs

- Doping Evolution of Antiferromagnetic Order and Structural Distortion in $LaFeAsO_{1-x}F_x$,

Q. Huang, J. Zhao, J. W. Lynn, G. F. Chen, J. L. Lou, N. L. Wang, and P. Dai, Phys. Rev. B **78,** 054529 (2008).

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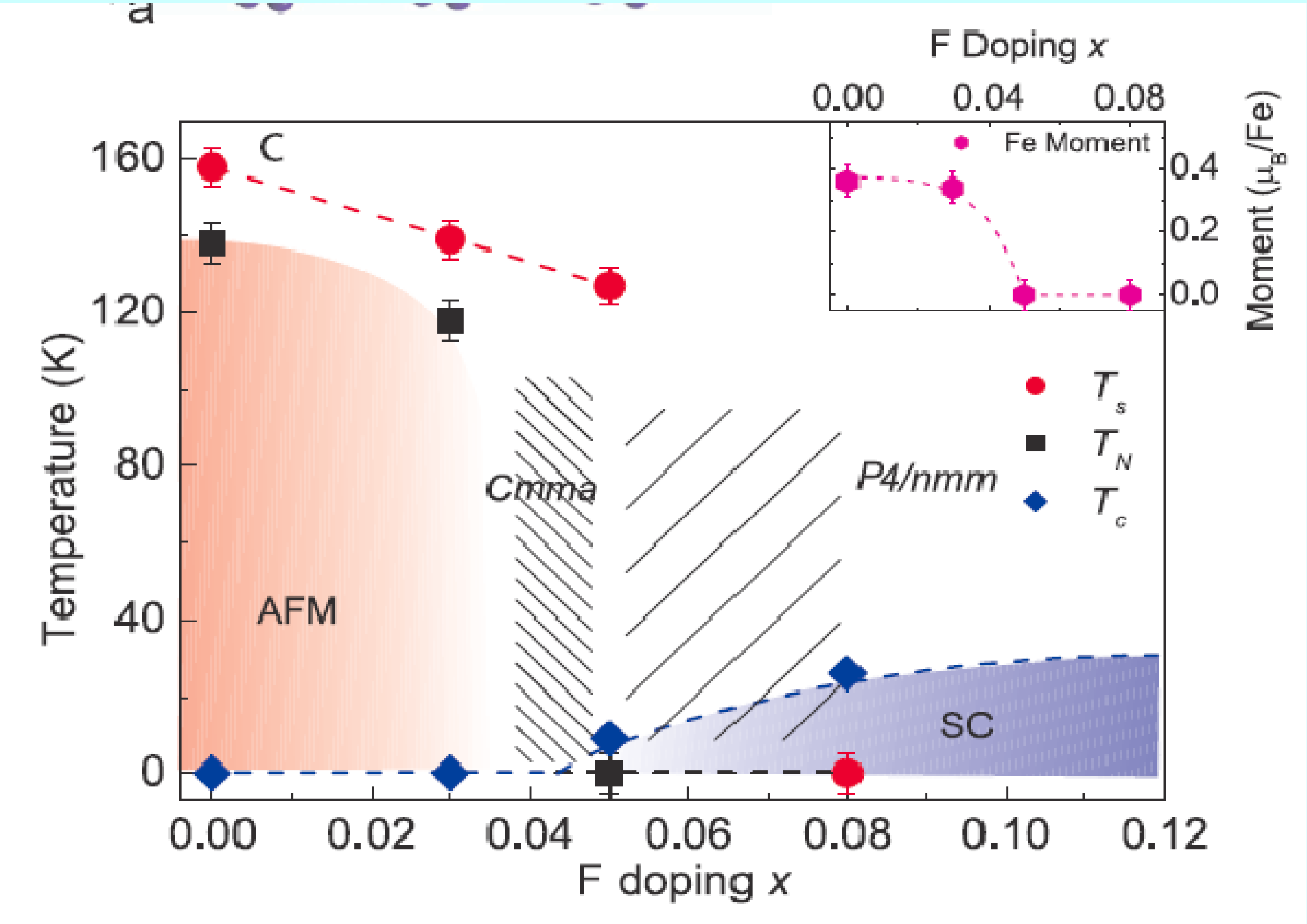
$LaFeAsO_{1-x}F_x$ Phase Diagram



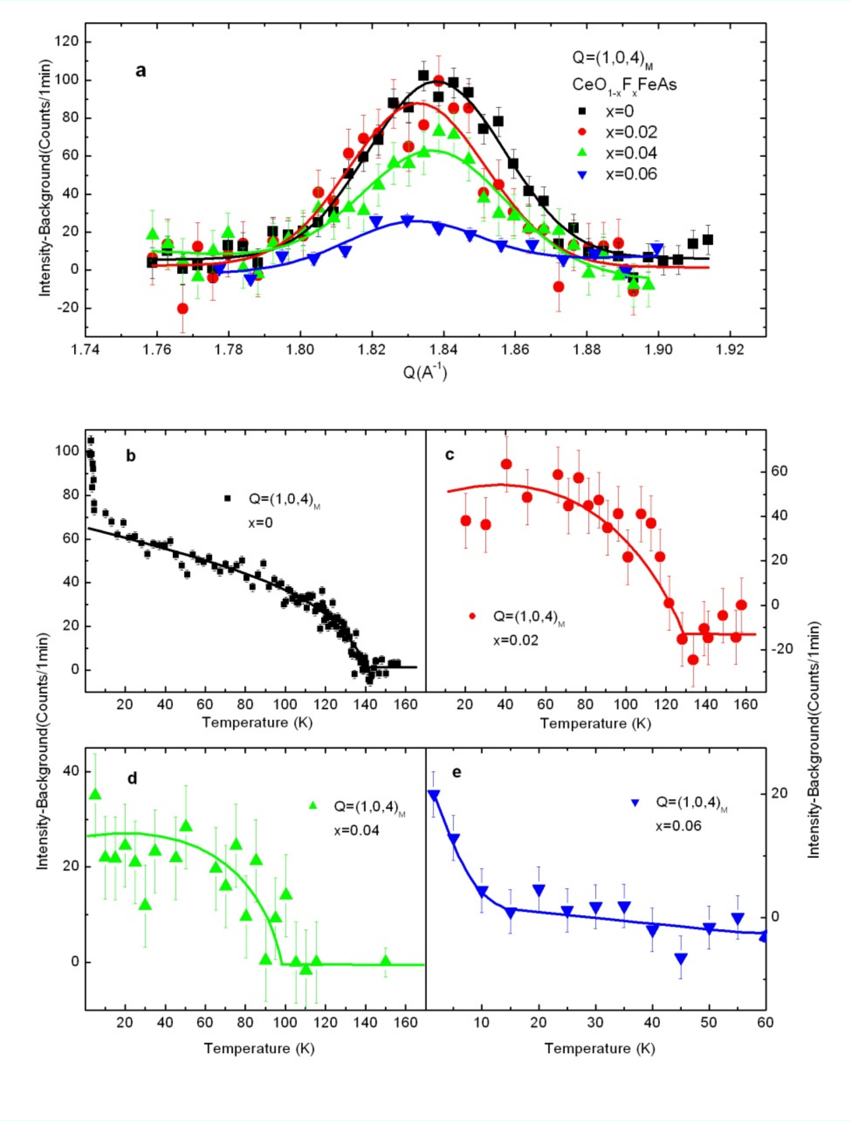
Doping Dependence of *Ce*(O,F)FeAs

- Structural and Magnetic Phase Diagram of $CeFeAsO_{1-x}F_x$ and its Relationship to High-Temperature Superconductivity,

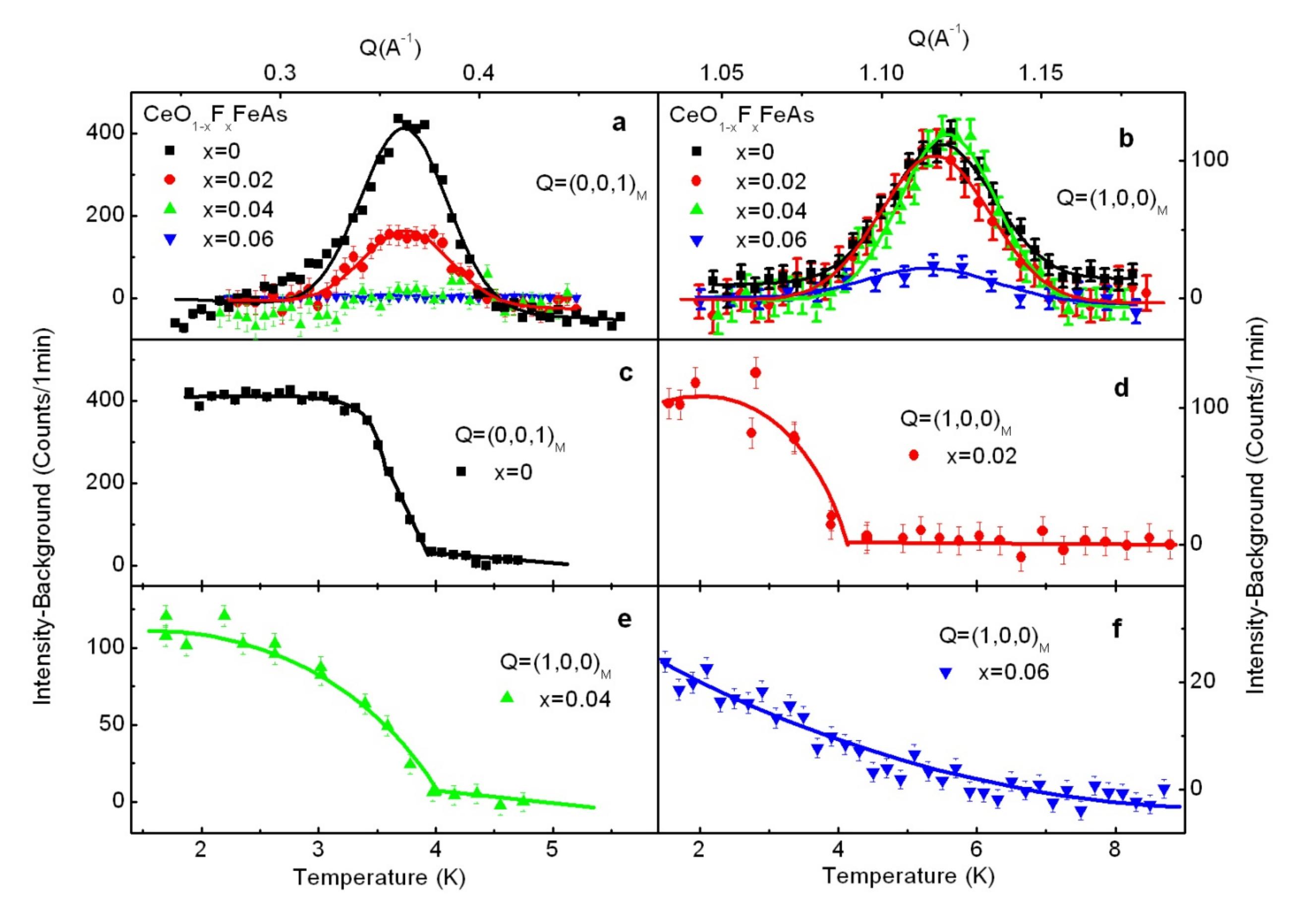
J. Zhao, Q. Huang, C. de al Cruz, S. Li, J. W. Lynn, Y. Chen, M. A. Green, G. F. Chen, G. Li, Z. C. Li, J. L. Luo, N. L. Wang, and P. Dai,

Nature Materials **7**, 953 (2008).

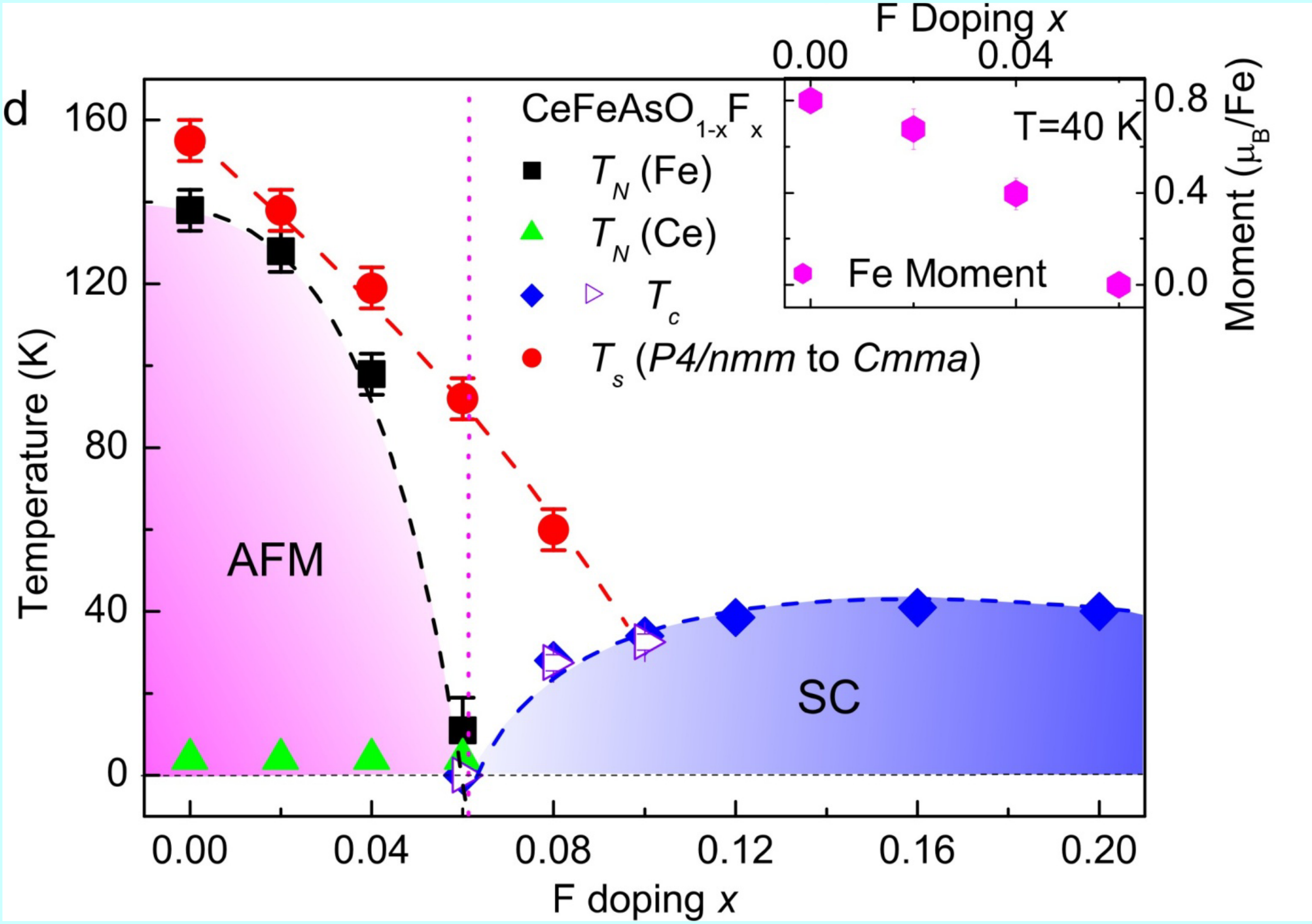
Fe Magnetic Structure of Ce(O,F)FeAs



Ce Magnetic Structure of Ce(O,F)FeAs

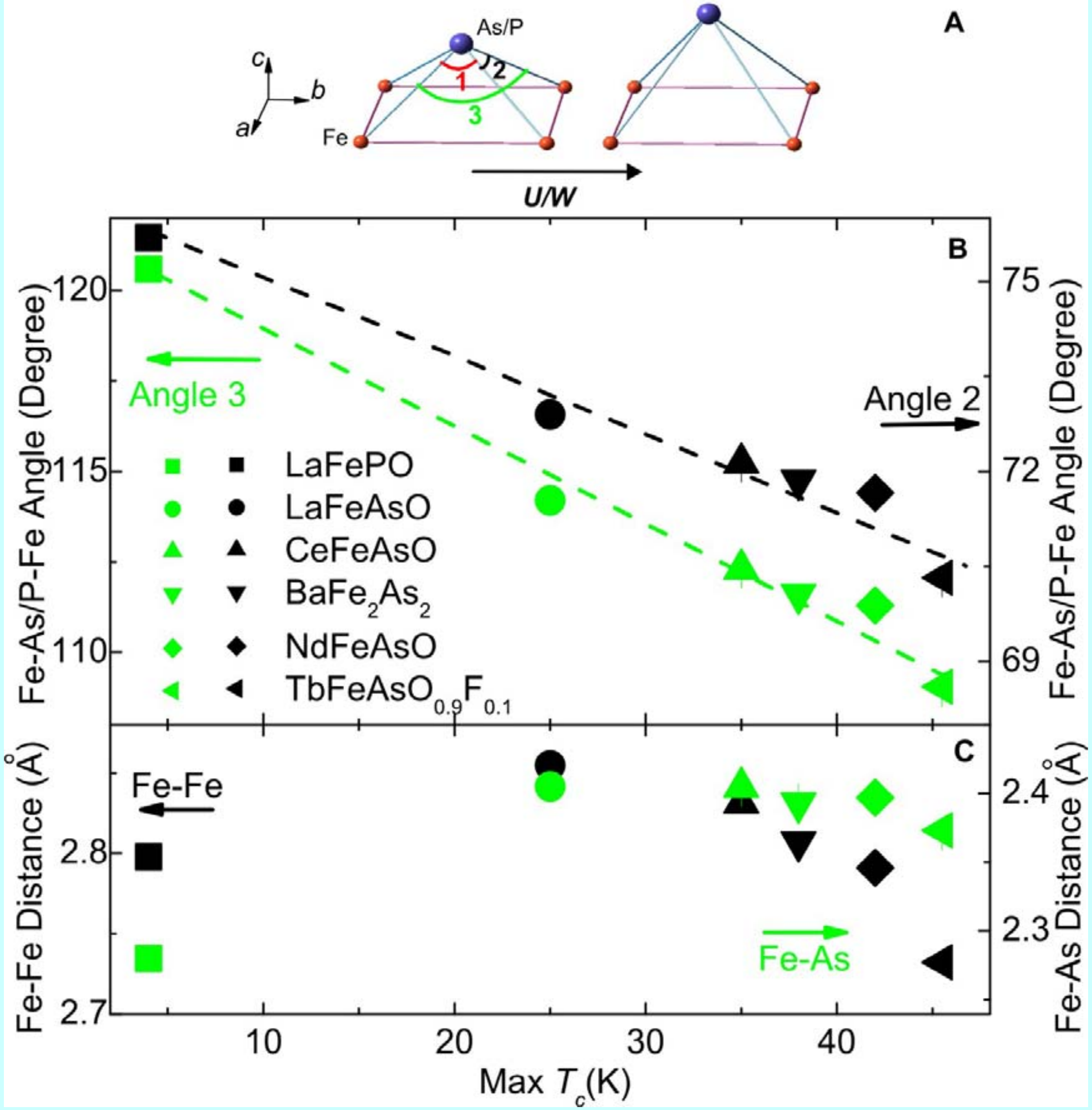


Phase Diagram of Ce(O,F)FeAs



J. Zhao**,** Q. Huang, C. de la Cruz, S. Li, J. W. Lynn, Y. Chen, M. A. Green, G. F. Chen, G. Li, Z. Li, J. L. Luo, N. L. Wang, and P. Dai, Nature Materials **7**, 953 (2008).

General T_C dependence for optimally doped *RE*(O,F)FeAs



Fe(Se-Te) Systems

First-order Magnetic and Structural Phase Transitions in $Fe_{1+y}Se_xTe_{1-x}$,
S. Li, C. de la Cruz, Q. Huang, Y. Chen, J. W. Lynn, J. Hu, Y-L Huang, F-C. Hsu, K-W. Yeh, M-K. Wu, and P. Dai, *Phys. Rev*. B **79**, 054503 (2009).

Incommensurate magnetic order in the alpha-Fe(Te,Se) superconductor systems
W. Bao, Y. Qiu, Q. Huang, M.A. Green, P. Zajdel, M.R. Fitzsimmons, M. Zhernenkov, M. Fang, B. Qian, E.K. Vehstedt, J. Yang, H.M. Pham, L. Spinu, Z.Q. Mao (submitted)

Extreme sensitivity of superconductivity to stoichiometry in $Fe_{1+x}Se$,
T. M. McQueen, Q. Huang, V. Ksenofontov, C. Felser, Q. Xu, H. Zandbergen, Y. S. Hor, J. Allred, A. J. Williams, D. Qu, J. Checkelsky, N. P. Ong, and R. J. Cava, Phys. Rev. B**79**, 014522 (2009).

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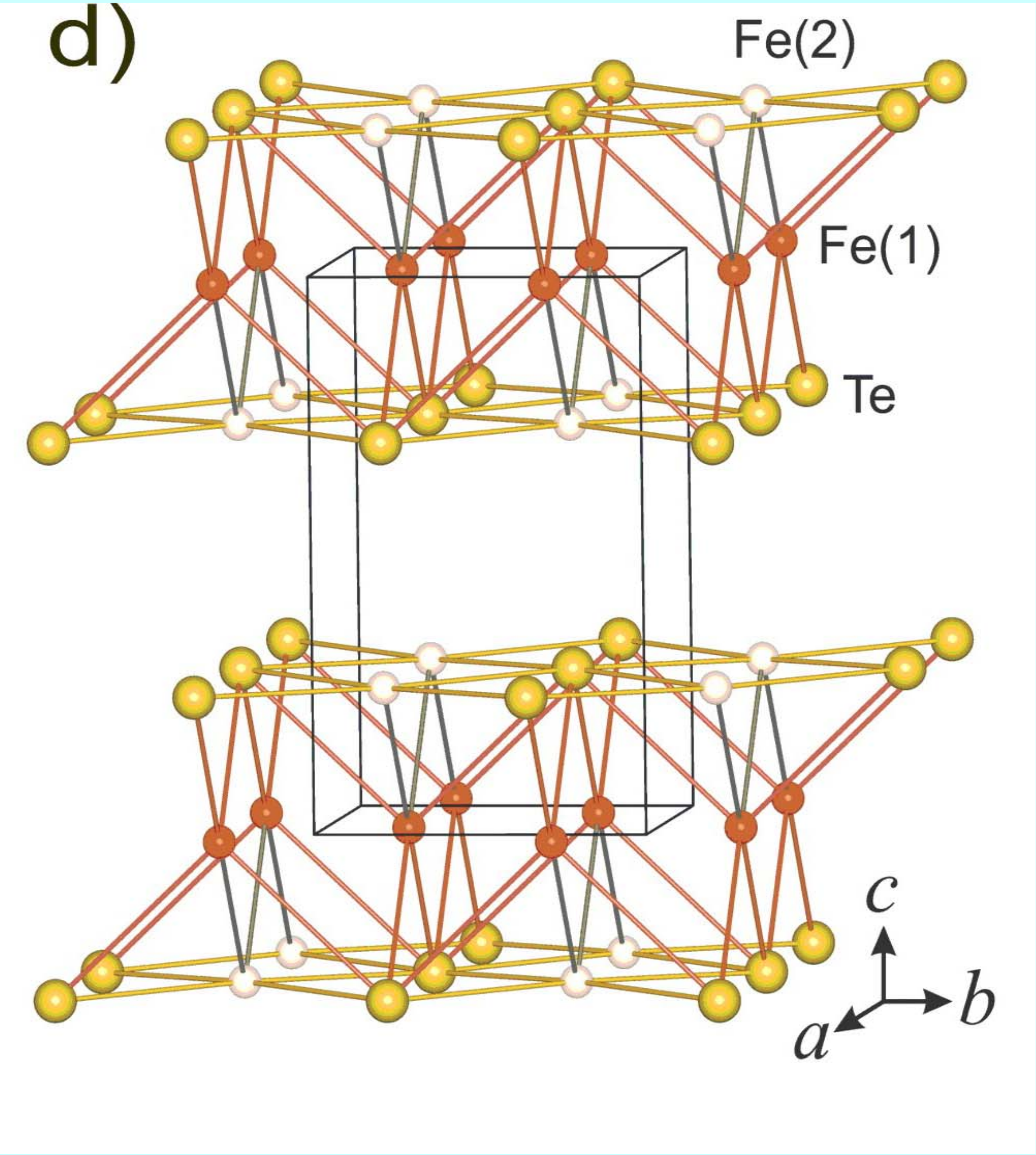


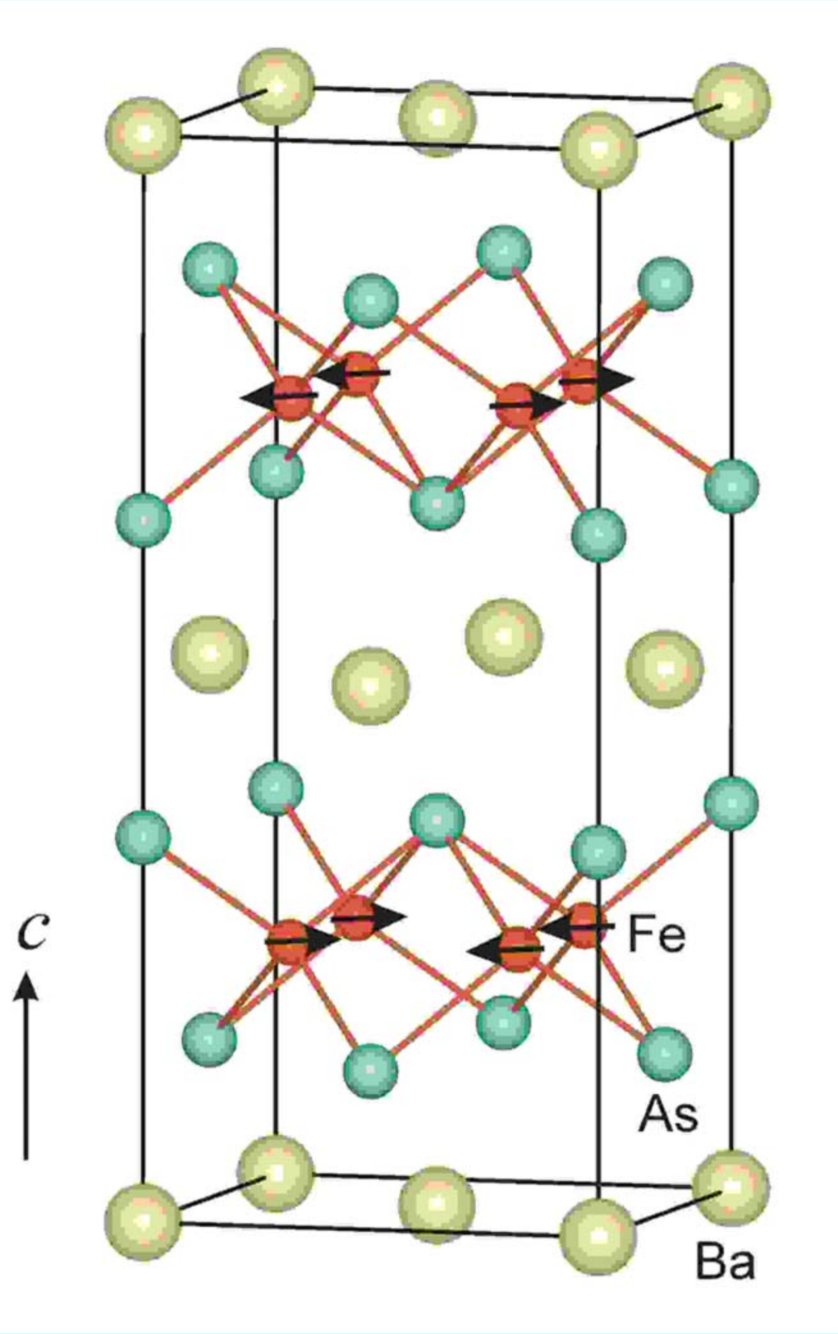
Crystal Structure [$Fe_{1.08}Te$]

Fe(Se-Te) Systems

$Fe_{1+x}Te$ Monoclinic:
Commensurate Antiferromagnetic for small x
Incommensurate antiferromagnet for larger x Different magnetic structure from 1:1:1:1 and 1:2:2 systems.

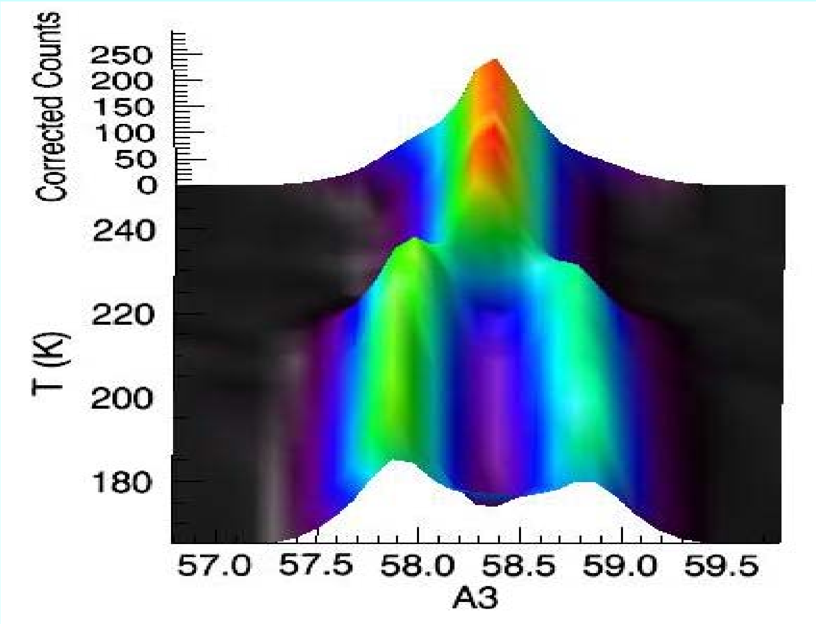
Fe_{1+x}(Te-Se) Orthorhombic superconductor with incommensurate magnetic correlations

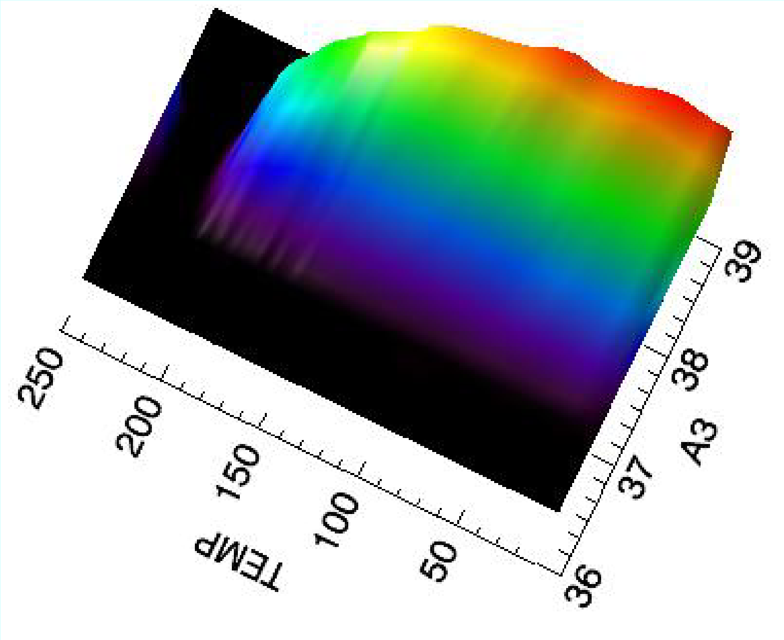
$(Ba, Ca, Sr)Fe_2As_2$ Systems

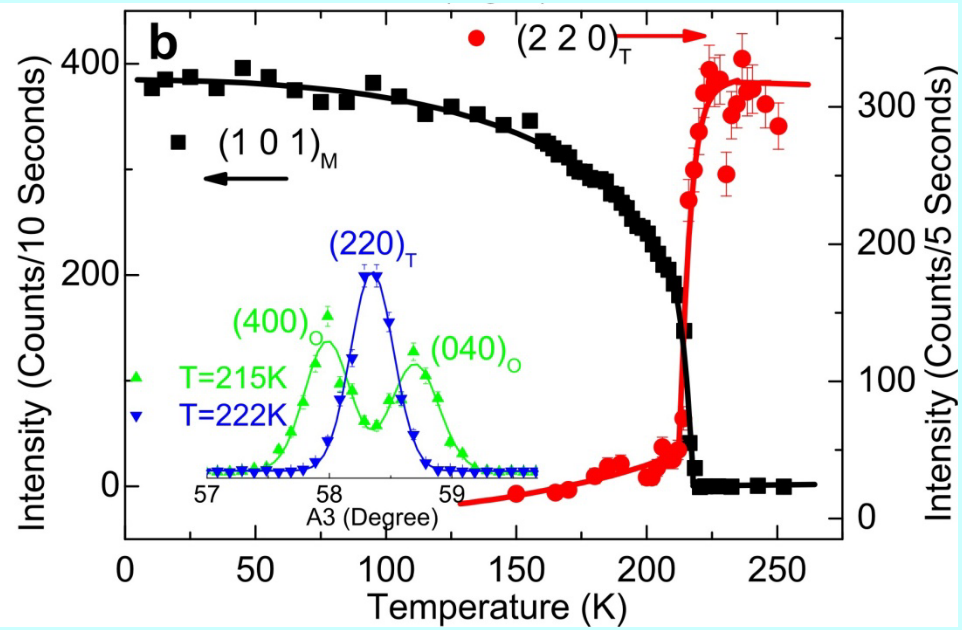


Magnetic and Crystal Structures of $(Ba,Sr,Ca)Fe_2As_2$

Single Crystal $SrFe_2As_2$







Spin and Lattice Structure of Single Crystal $SrFe_2As_2$, Jun Zhao, W. Ratcliff-II, J. W. Lynn, G. F. Chen, J. L. Luo, N. L. Wang, Jiangping Hu, and Pengcheng Dai, Phys. Rev. B **78,** 140504(R) (2008).

NIST Center for Neutron Research DAVE Data Analysis and Visualization Environment

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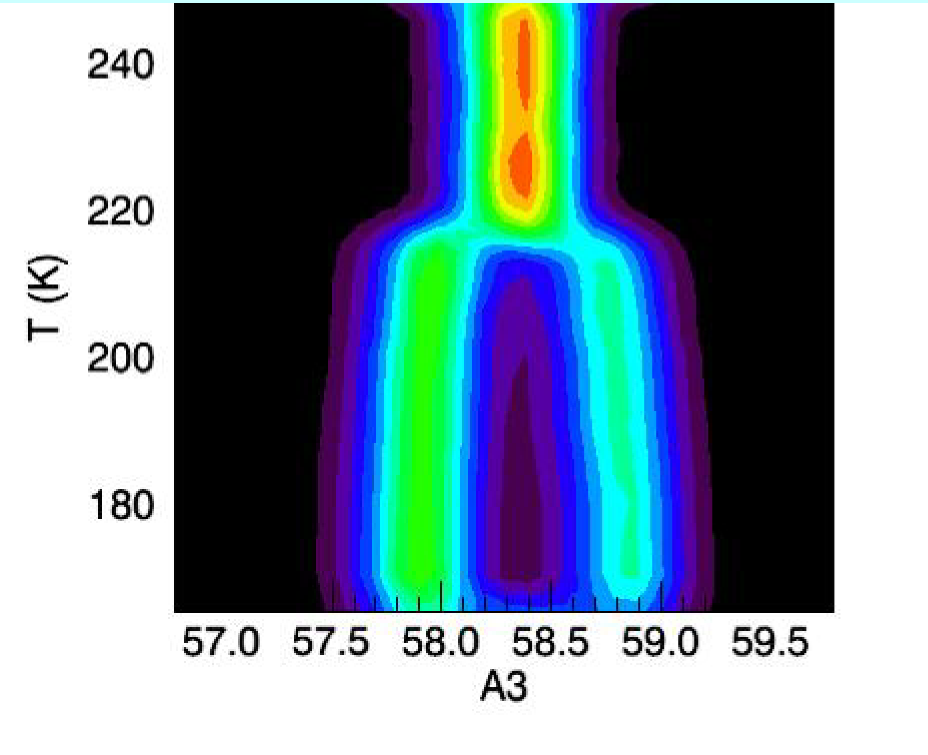
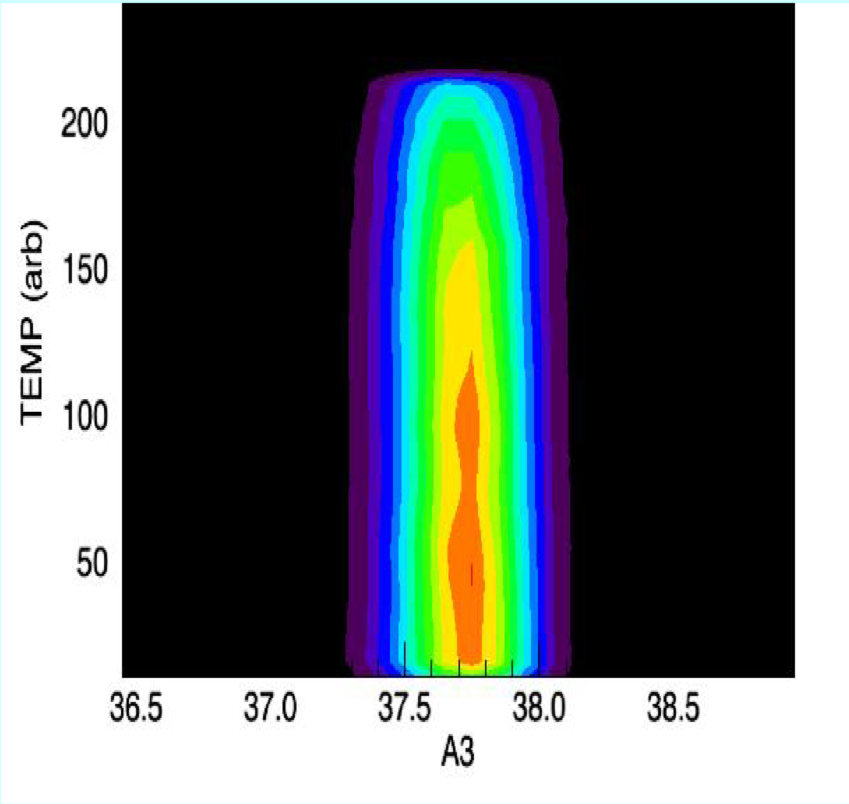
$SrFe_2As_2$



Structure

Magnetic



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DAVE
Data Analysis and Visualization Environment

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$CaFe_2As_2$ System

- Pressure-induced volume-collapsed Tetragonal Phase of $CaFe_2As_2$ as seen via Neutron Scattering, A. Kreyssig, M. A. Green, Y. B. Lee, G. D. Samolyuk, P. Zajdel, J. W. Lynn, S. L. Bud'ko, M. S. Torikachvili, N. Ni, S. Nandi, J. Leão, S. J. Poulton, D. N. Argyriou, B. N. Harmon, P. C. Canfield, R. J. McQueeney, and A. I. Goldman, Phys. Rev. B**78**, 184517 (2008).
- Lattice Collapse and Quenching of Magnetism in $CaFe_2As_2$ under Pressure: A Single Crystal Neutron and X-ray Diffraction Investigation, A. I. Goldman, A. Kreyssig, K. Prokes, D. K. Pratt, D. N. Argyriou, J. W. Lynn, S. Nandt, S. A. Kimber, Y. Chen, Y. B. Lee, G. Samolyuk, J. Leao, S. J. Poulton, S. L. Bud'ko, N. Ni, P. C. Canfield, B. N. Harmon, and R. J. McQueeney, *Phys. Rev*. B**79**, 024513 (2009).

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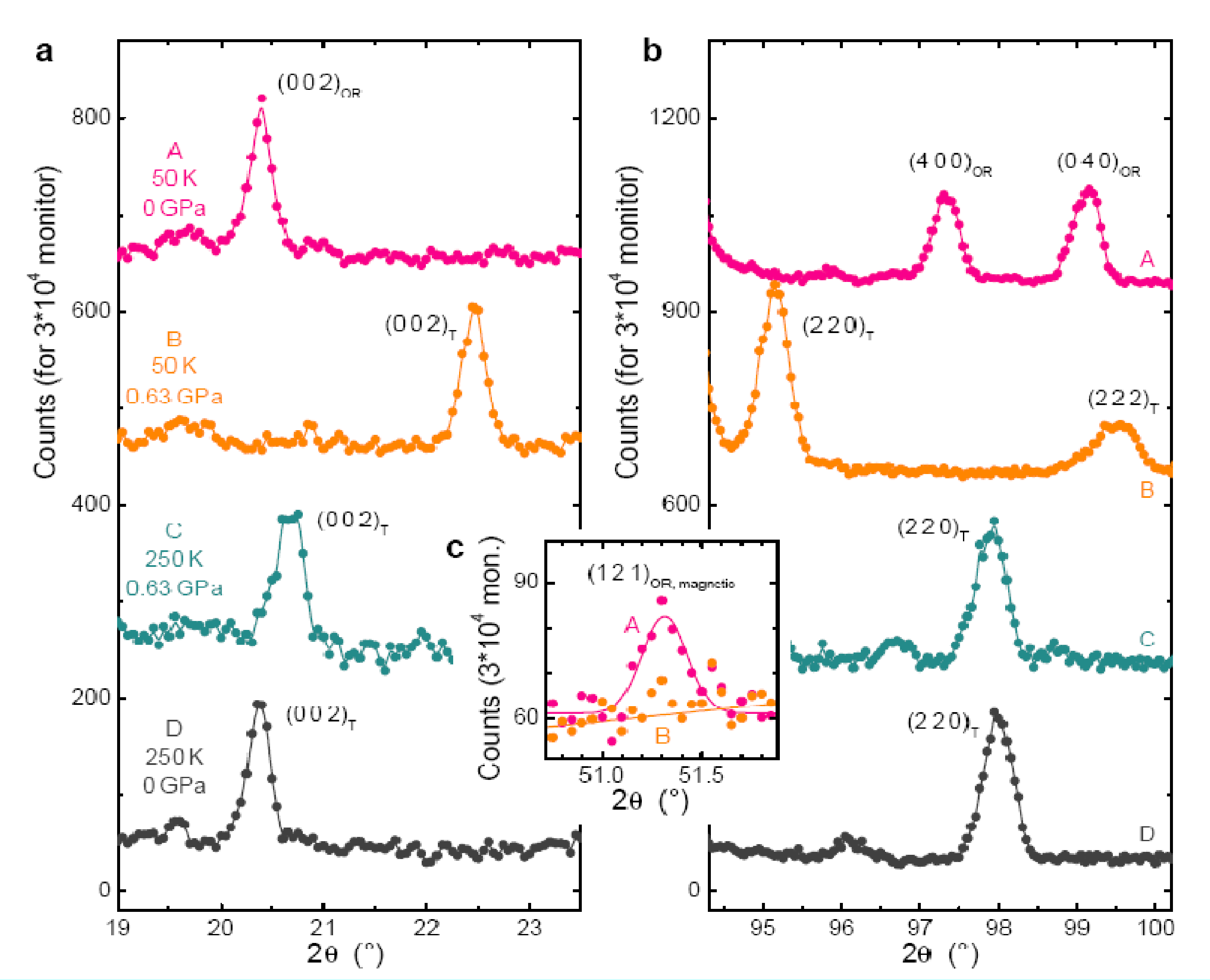
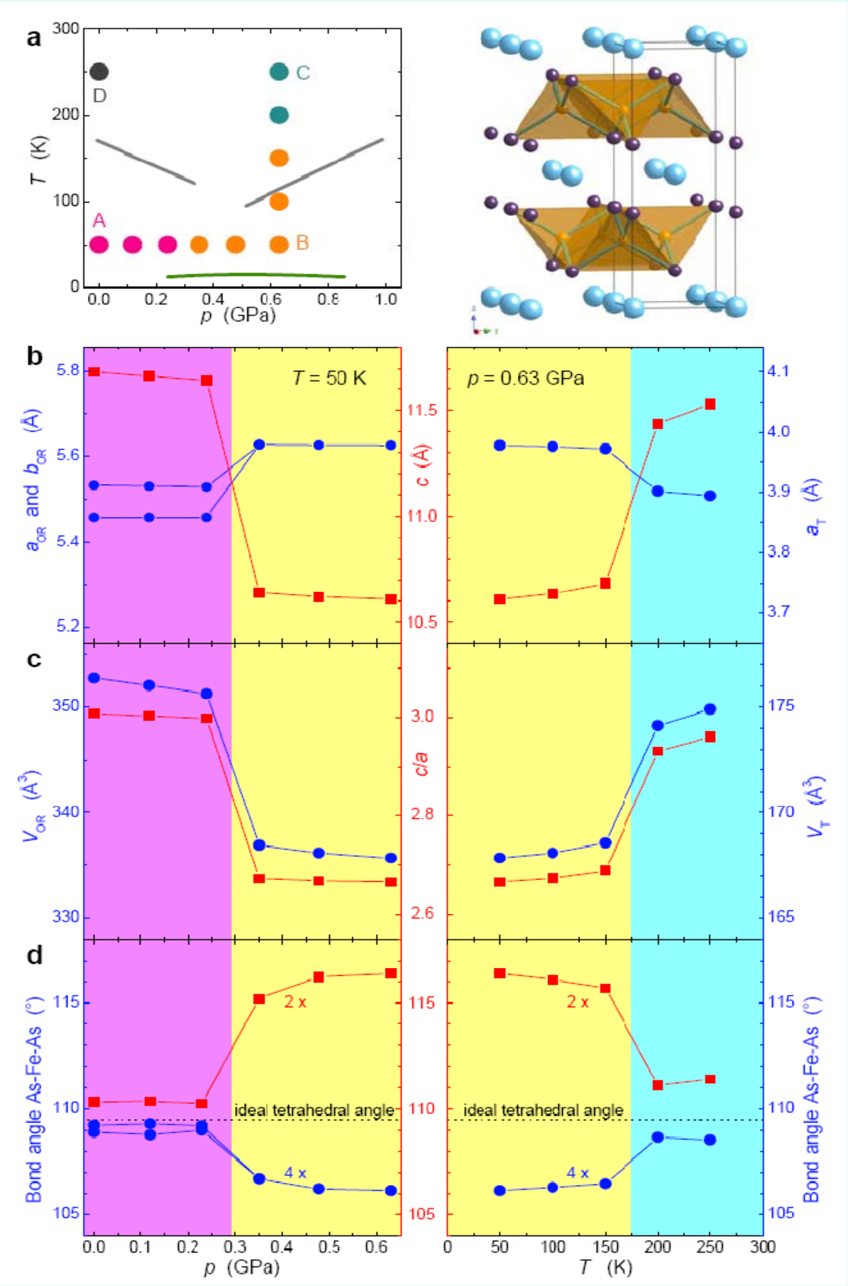
$CaFe_2As_2$



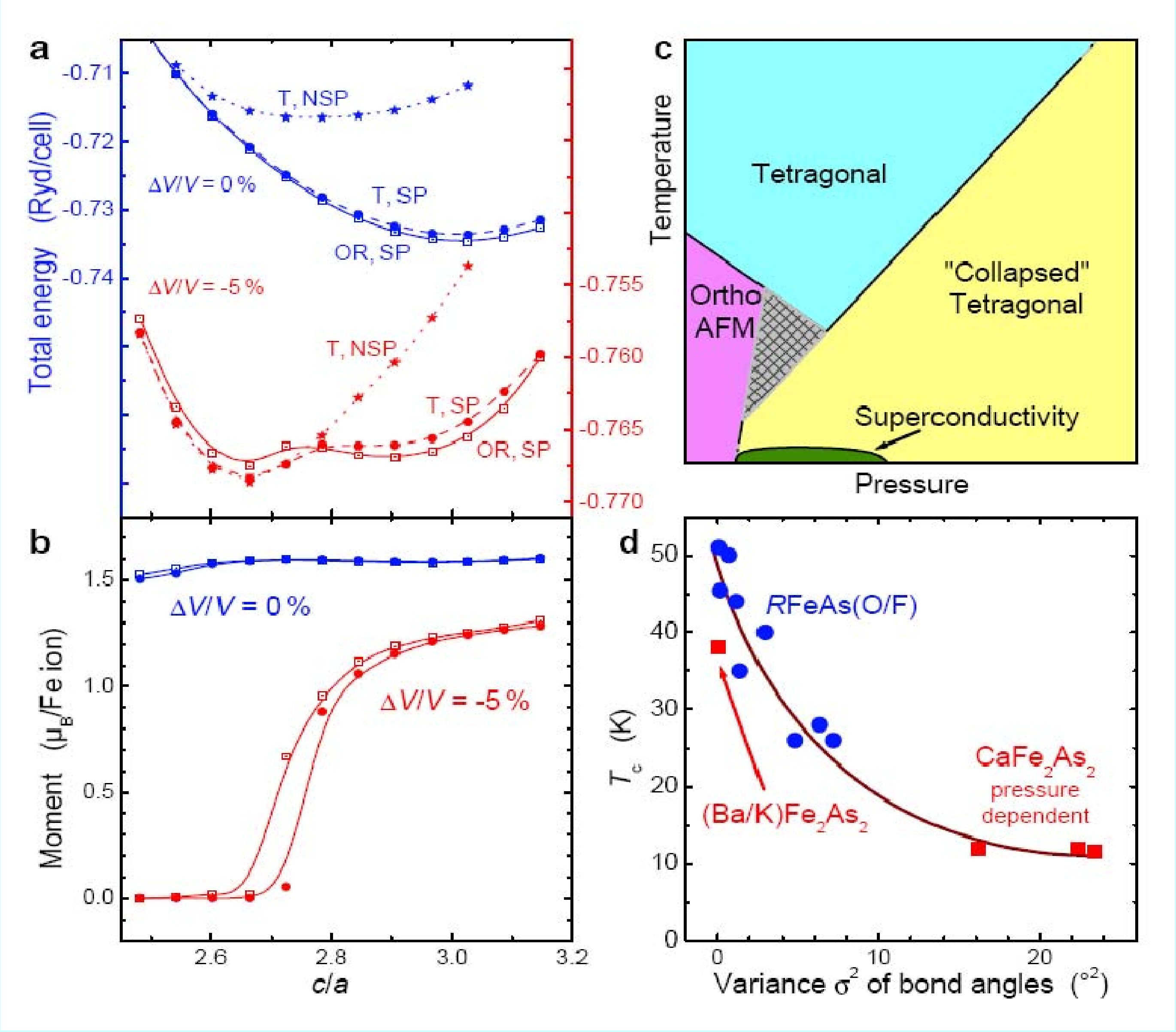
a
b
c
(0 0 2)OR
A
50 K
0 GPa
B
50 K
0.63 GPa
(0 0 2)T
C
250 K
0.63 GPa
D
250 K
0 GPa
Counts (for 3*10^4 monitor)
2θ (°)
(4 0 0)OR
(0 4 0)OR
(2 2 0)T
(2 2 2)T
(1 2 1)OR, magnetic
Counts (3*10^4 mon.)

$CaFe_2As_2$



a
T (K)
p (GPa)
D
C
A
B
b
T = 50 K
p = 0.63 GPa
a_OR and b_OR (Å)
c (Å)
a_T (Å)
c
V_OR (Å³)
c/a
V_T (Å³)
d
Bond angle As-Fe-As (°)
2 x
4 x
ideal tetrahedral angle
p (GPa)
T (K)

$CaFe_2As_2$



NCNR

Inelastic Scattering
Spin Waves

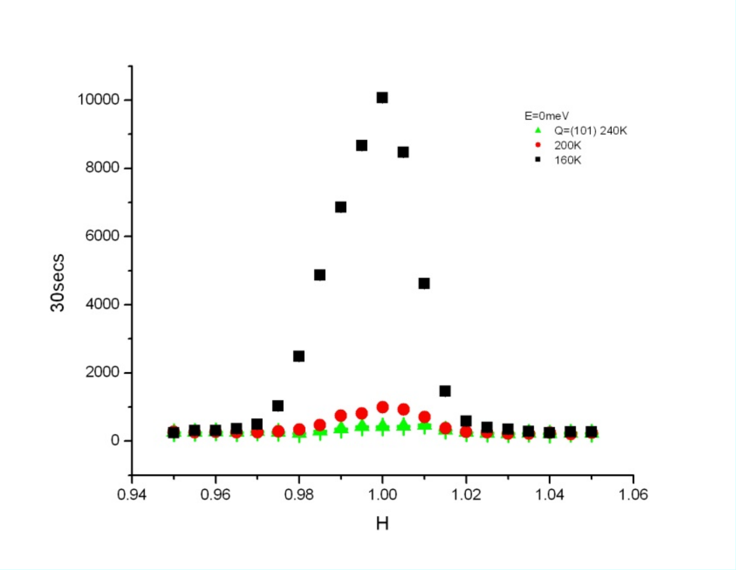
Low energy spin waves and magnetic interactions in SrFeAs,

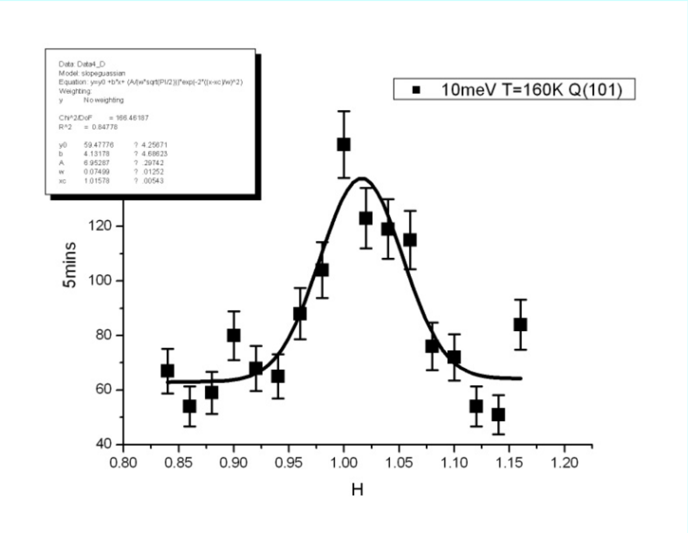
Jun Zhao, Dao-Xin Yao, S. Li, Tao Hong, Y. Chen, S. Chang, W. Ratcliff II, J. W. Lynn, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, E. W. Carlson, J. Hu, and P. Dai,

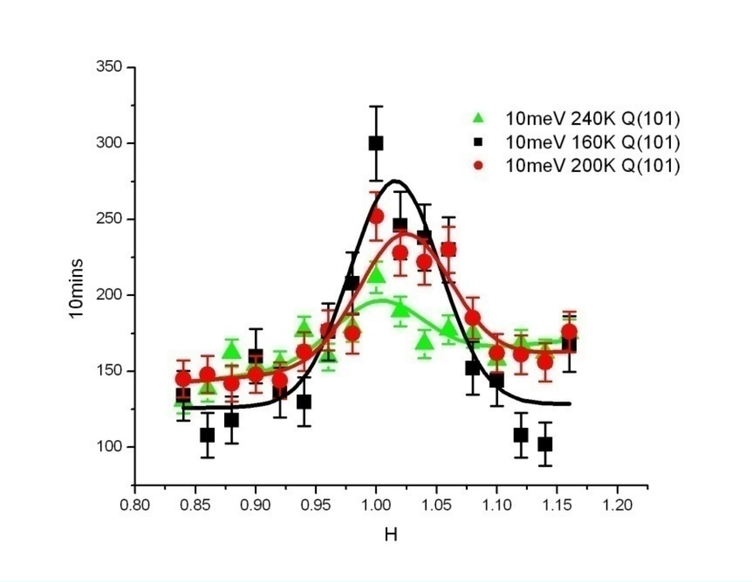
Phys. Rev. Lett. **101**, 167203 (2008).

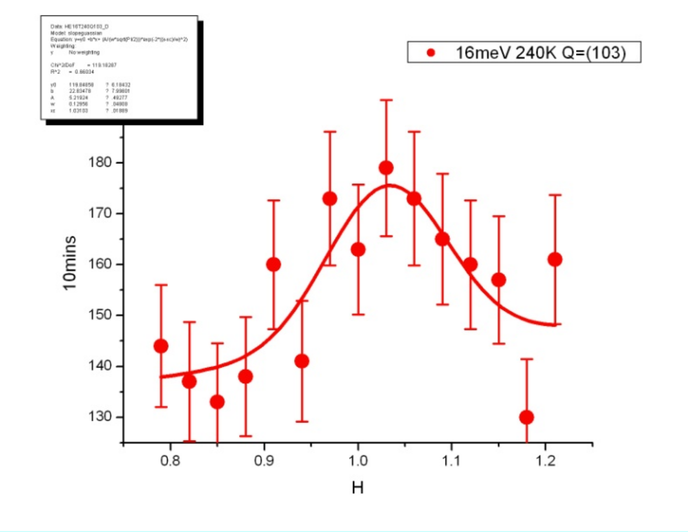
NCNR

Spin Waves In $SrFe_2As_2$









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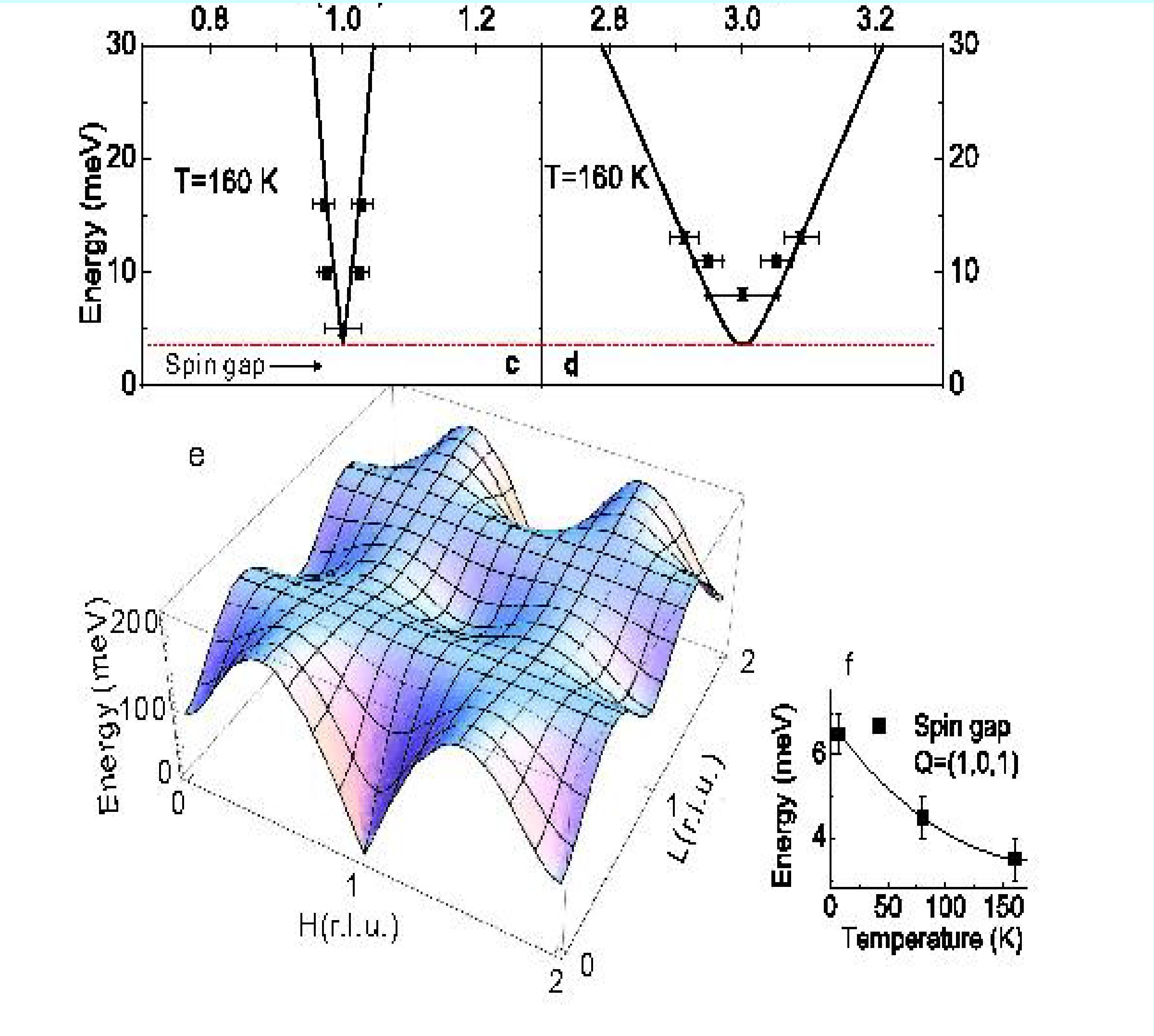
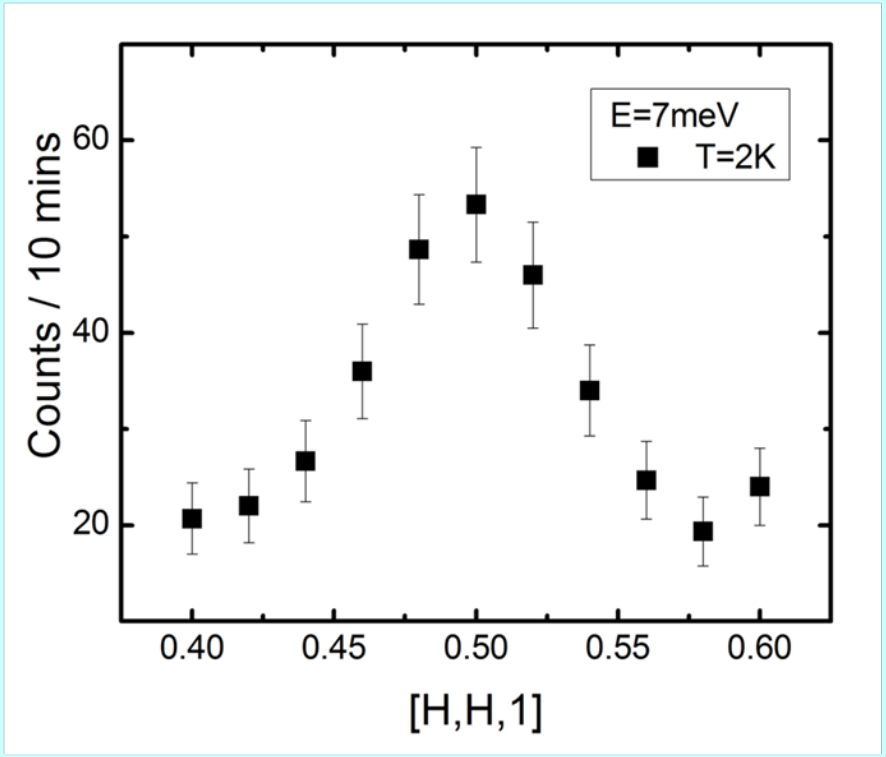
Spin Waves In $SrFe_2As_2$

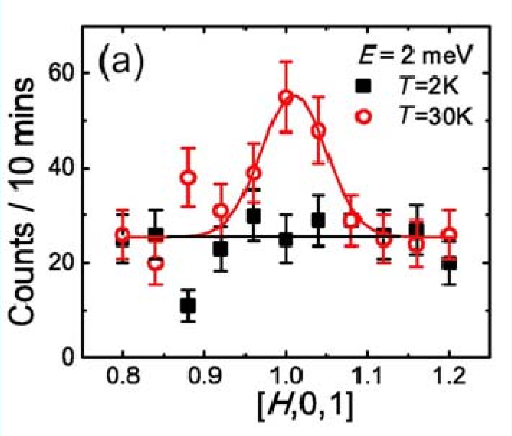


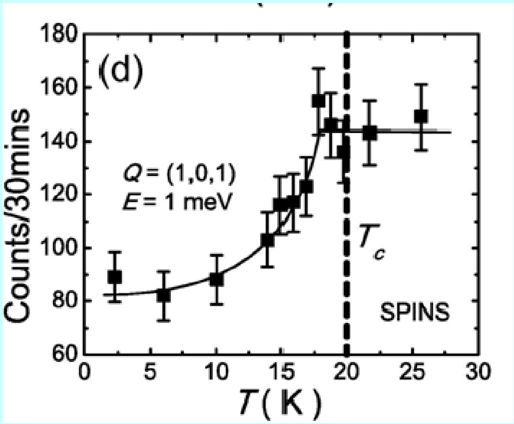
Jun Zhao, Dao-Xin Yao, S. Li, Tao Hong, Y. Chen, S. Chang, W. Ratcliff II, J. W. Lynn, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, E. W. Carlson, J. Hu, and P. Dai, Phys. Rev. Lett. **101**, 167203 (2008).

Spin Excitations In Superconducting $BaFe_{1.9}Ni_{0.1}As_2$



Resonance Energy

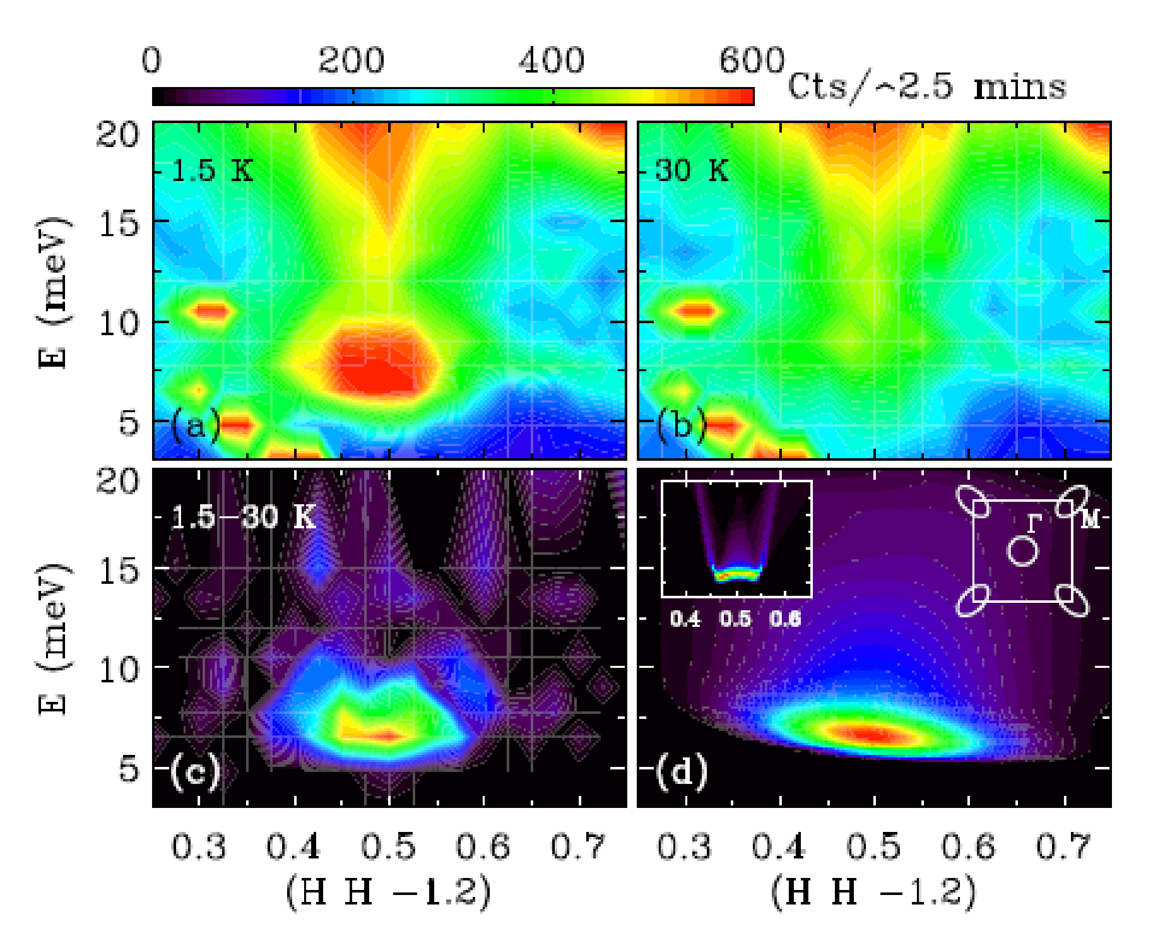




Spin Gap

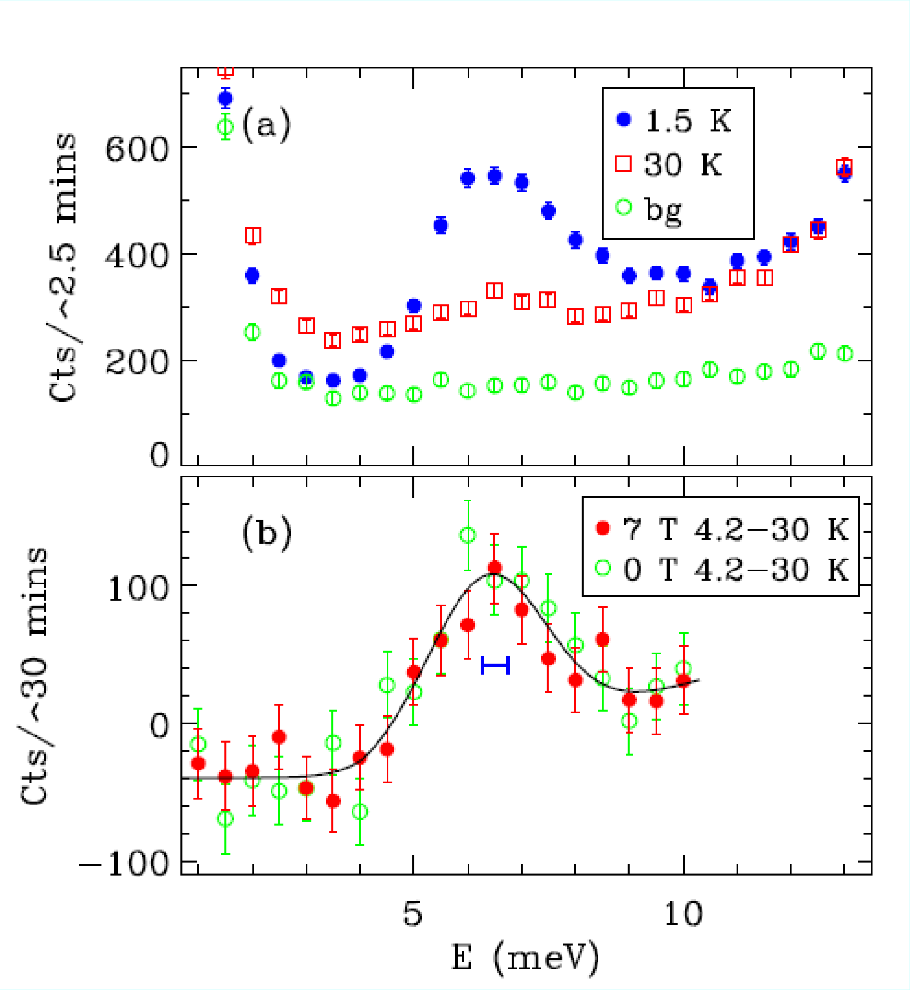
S. Li, Y. Chen, S. Chang, J. W. Lynn, L. Li, Y. Luo, G. Cao, Z. Xu, P. Dai, Phys. Rev. B **79**, 054503 (2009).

Spin Resonance in $Fe(Se_{0.4}Te_{0.6})$



Y. Qiu, W. Bao, Y. Zhao, C. Broholm, V. Stanev, Z. Tesanovic, Y.C. Gasparovic, S. Chang, J. Hu, B. Q., M. Fang, and Z. Mao, arXiv:0905.3559

Spin Resonance in Fe($Se_{0.4}Te_{0.6}$)



Y. Qiu, W. Bao, Y. Zhao, C. Broholm, V. Stanev, Z. Tesanovic, Y.C. Gasparovic, S. Chang, J. Hu, B. Q., M. Fang, and Z. Mao, arXiv:0905.3559

Overall Summary

- Magnetic Superconductors have a rich and interesting history, ranging from "***shouldn't have magnetic spins in the lattice***" to "***must have magnetic spins in the lattice***"
- For Cuprate Superconductors, the Cu spin dynamics provide the needed high energy scale. The magnetic resonance is directly tied to the superconducting state for both hole and electron-doped cuprates.
- the iron-based superconductors exhibit a similar phase diagram to the cuprates. The 'parent' systems exhibit a ubiquitous structural transition, below which long range antiferromagnetic occurs. The magnetic energetics is ~200 meV, also similar to the cuprates. The role of spin fluctuations in the superconducting pairing is clear

Review:

Neutron Studies of the Iron-based Family of High Tc Magnetic Superconductors, J. W. Lynn and Pengcheng Dai, Physica C**469**, 469 (2009).

List of publications at http://www.ncnr.nist.gov/staff/jeff

Instrument Publications (TAS spectrometers, DCS, BT-1)