17. Neutron Inelastic Scattering Study on Superconducting and Parent Phases of the $Ba(Fe,Co)_2As_2$ System

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We will report recent results of single-crystal growth and inelastic neutron scattering measurements on superconducting $Ba(Fe,Co)_2As_2$ and its parent compound $BaFe_2As_2$. For both the systems, large single crystals of the typical size $10x4x2mm^3$ were obtained using the vertical Bridgman technique [1]. In the parent compound, inelastic neutron scattering using single-crystals reveals a spin-wave-like excitation mode centered at the antiferromagnetic Bragg points with the gap energy being 9.8 meV at the base temperature [2]. The spin-wave-like mode has a steep in-plane dispersion with a velocity 280 meV Å, whereas relatively weak dispersion was seen along the *c*-axis. In addition, a two-dimensional excitation continuum appears at higher energies $\hbar\omega > 20$ meV, suggesting electron-hole excitations in this energy range. As the temperature is elevated, the excitation gap closes, and above the Neel temperature, gapless spin fluctuations of much two-dimensional nature dominate the excitation spectrum. The inelastic response in the superconducting phase will be also presented.

References

[1] R. Morinaga, K. Matan, H. S. Suzuki, and T. J. Sato, Jpn. J. Appl. Phys. (in press) (arXiv:0809.3084).
[2] K. Matan, R. Morinaga, K. Iida, and T. J. Sato (submitted) (arXiv: 0810.4790).

Inelastic Neutron Scattering Measurements on Single Crystal $BaFe_2As_2$

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International Workshop on Iron Related High-T_c Superconductors

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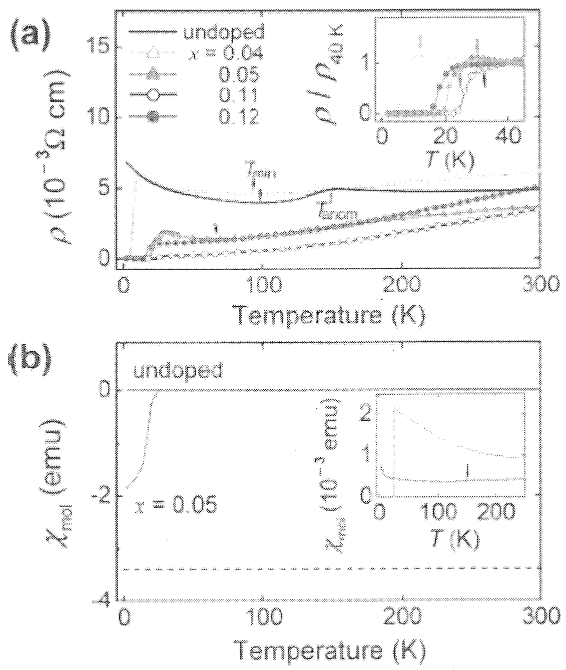
R. Morinaga et al., Jpn. J. Appl. Phys. 48, 013004 (2009)
K. Matan, et al., arXiv:0810.4790

Outline

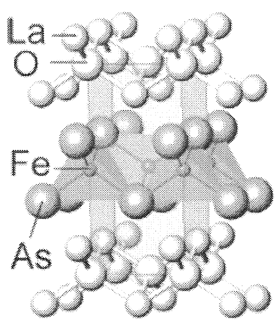
- ☆ Magnetism in FeAs compounds
- ☆ Inelastic neutron scattering on single-crystal $BaFe_2As_2$
- ☆ Spin fluctuations above T_N
- ☆ Preliminary results on superconducting sample
- ☆ Summary

Superconductivity in F-doped LaFeAsO

Kamihara et al., J. Am. Chem Soc. 130, 3296 (January 2008)



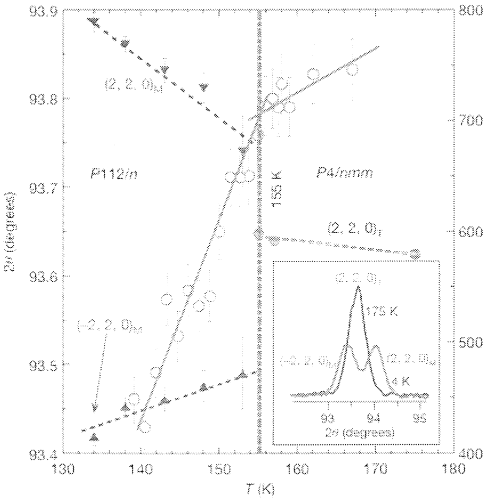
- Parent compounds are poor metals.
- Electron-doped $LaFeAsO_{1-x}F_x$ with T_c of ~26 K.
- Hole-doped $La_{1-x}Sr_xFeAsO$ with T_c of ~25 K.
- Changing of La to rare earth ions results in T_c ~ 52 K.

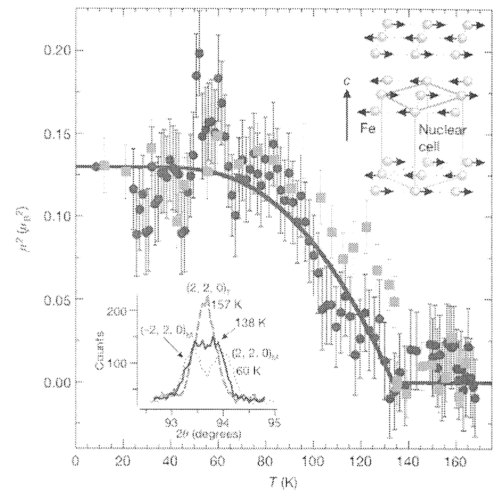


What is the anomaly around 150K?

Structural and magnetic transitions in LaFeAsO

de la Cruz et al., Nature 453, 899 (June 2008)





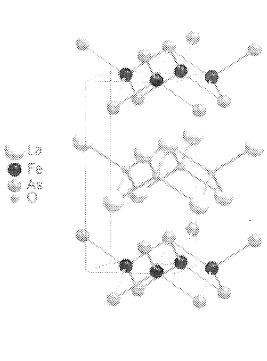
Structural transition at 155 K

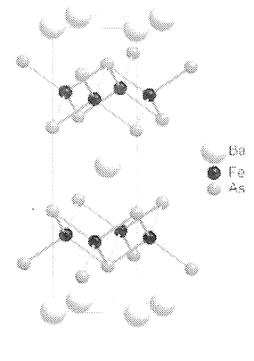
Magnetic transition at ~138 K

The discovery of LaFeAsO led to discoveries of many other Fe-based superconductors.

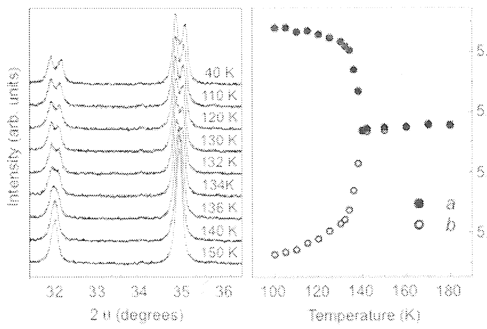
Structural and magnetic transitions in $BaFe_2As_2$

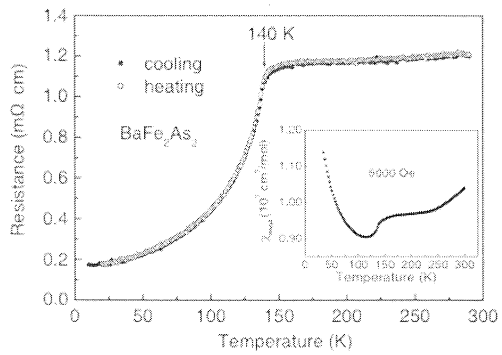
Rotter et al., Phys. Rev. B. 78, 020503 (July 2008)





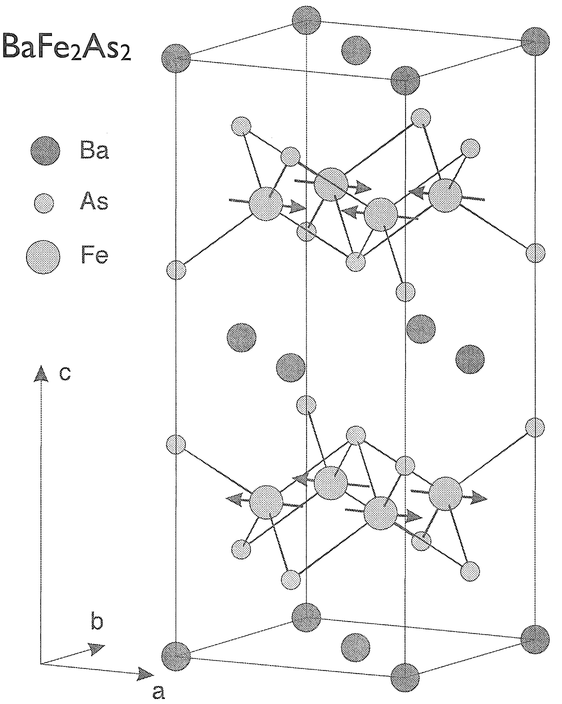
- Similar structure, and electronic-magnetic properties.
- Antiferromagnetic and structural transitions at T_N ~135 K.
- Superconductivity in K, Co, Cs, Ni doped AFe_2As_2, A=Ba, Sr, Ca, and Eu with the highest T_c of 38 K.





Magnetism and superconductivity in $BaFe_2As_2$

$BaFe_2As_2$



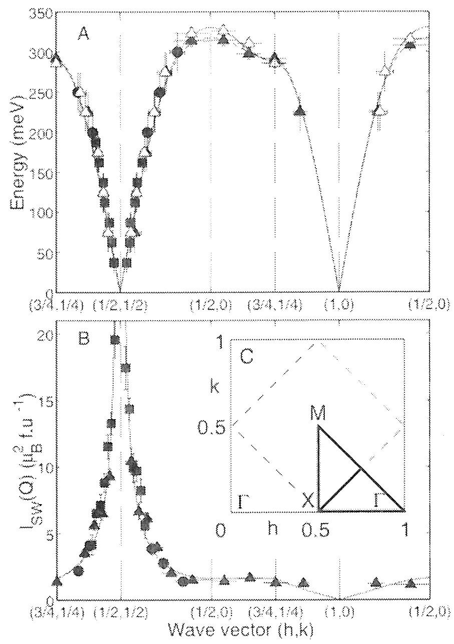
- Powder neutron diffraction reveals antiferromagnetic spin structure in FeAs layers with an ordered moment of $0.87(3)\ \mu_B$.
  (Huang et al., Phys. Rev. Lett. 101, 257003)
- Magnetic order is a result of SDW instability due to Fermi surface nesting.
  (Mazin et al., Phys. Rev. Lett. 101, 057003)
- Magnetic ordered state is suppressed by doping or pressure.
- The suppression of magnetic ordered state is accompanied by the presence of superconductivity.

Itinerant magnetism

Magnetic excitations in parent compounds

La_2CuO_4

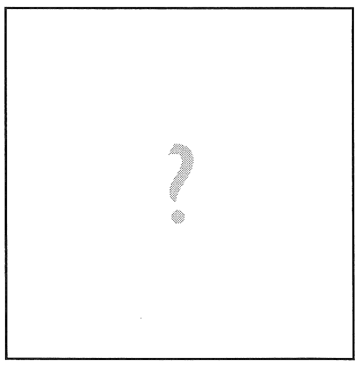
Localized spins



Coldea et al., Phys. Rev. Lett. 86, 5377 (2001)

$BaFe_2As_2$

Itinerant spins



- Low energy spin wave excitations.
- Electron-hole excitations at high energy (the Stoner continuum).

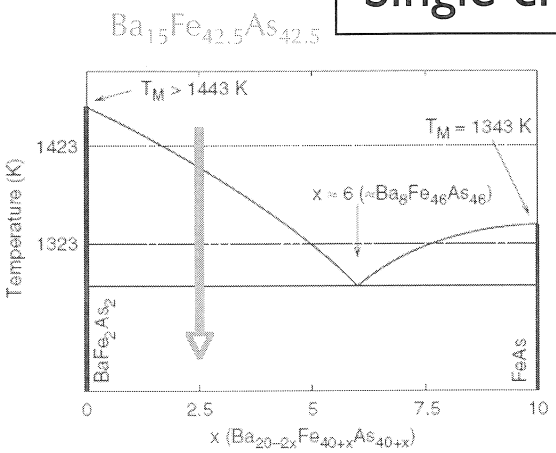
Goals

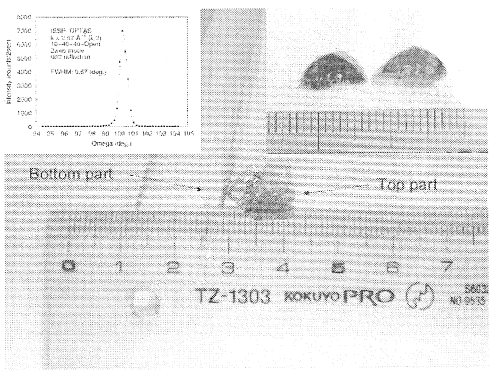
I. To study anisotropic magnetic interactions; excitations and spin fluctuations.

II. Investigate itinerant magnetism, signature of the Stoner continuum.

Magnetic excitation studies using inelastic neutron scattering measurements on a single crystal sample.

Single crystal growth





Morinaga et al., arXiv:0809.3084 (Jpn. J. Appl. Phys. in press)

Single-crystal sample

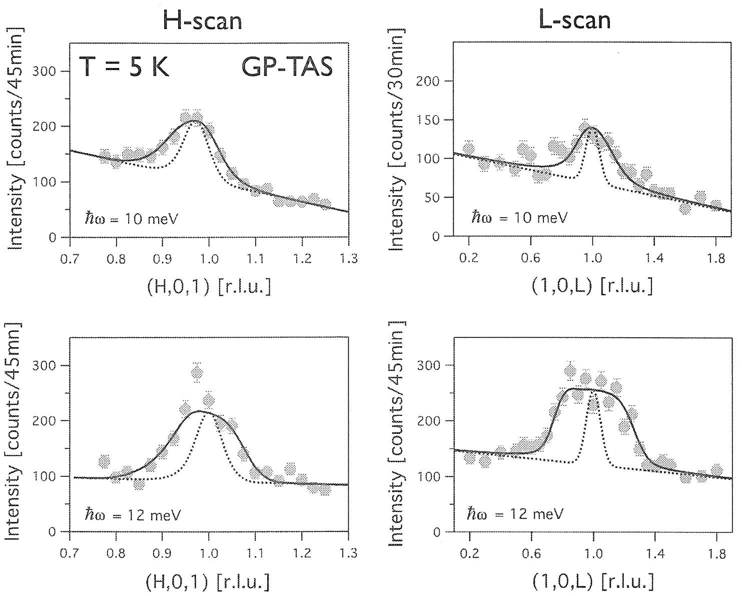
- The sample was grown in our ISSP lab.
- Bridgman method using FeAs flux.
- Size ~10mm x 5mm x 2mm.

Neutron scattering measurements

- Two co-aligned single crystals M=0.4 g
- Mosaic < 1°
- HER and GP-TAS (ISSP, U. of Tokyo)
- Aligned in *h0l* zone a* = 1.124(3) Å^{-1} and c* = 0.485 Å^{-1}.

Large enough single crystals to perform inelastic neutron scattering.

Low energy spin-wave-like excitations

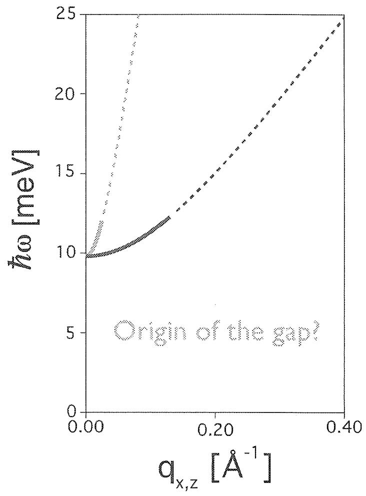


Δ = 9.8(4) meV

v_{ab} = 280(150) meV

v_c = 57(7) meV

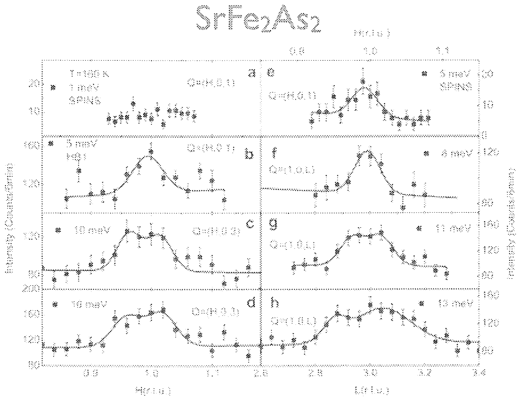
$v_c/v_{ab} \sim 0.2$



Empirical dispersion relation

Spin wave excitations in $SrFe_2As_2$ and $CaFe_2As_2$

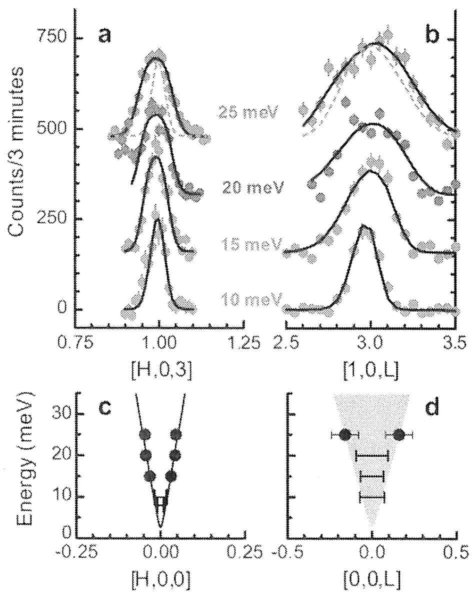
$SrFe_2As_2$



Zhao et al., Phys. Rev. Lett. 101, 167203 (2008)

$SrFe_2As_2$	$CaFe_2As_2$
$\Delta \leq$ 6.5 meV	Δ = 6.9(2) meV
v_{ab} = 560 meV	v_{ab} = 420(70) meV
v_c = 280 meV	v_c = 270(100) meV

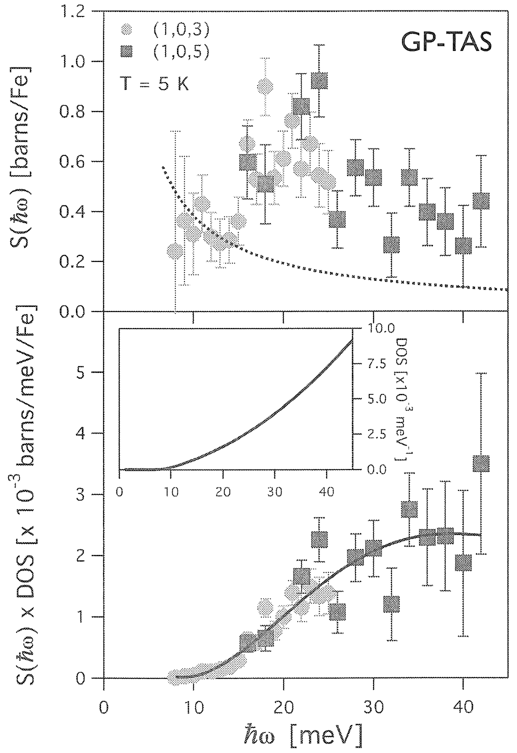
$CaFe_2As_2$



McQueeney et al., Phys. Rev. Lett. 101, 227205 (2008)

Magnetic interactions in $BaFe_2As_2$ are more two-dimensional.

High energy magnetic excitations

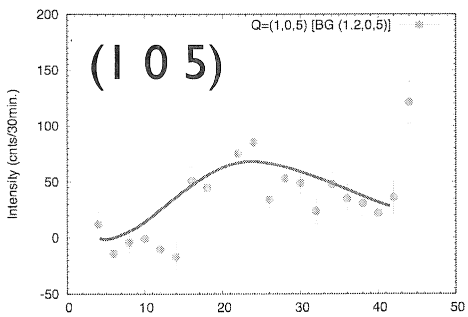


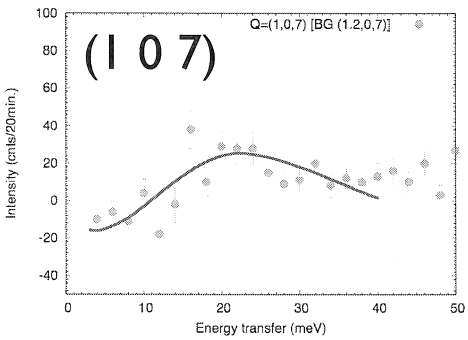
- Normalization function obtained from acoustic phonons of copper
- Corrected for background, absorption, resolution, and magnetic form factor.
- For ħω < 15 meV, S(ħω) shows the 1/ω dependence for spin wave scattering.
- For ħω > 15 meV, S(ħω) deviates from spin wave at 15 meV, and peaks around 20 meV.
- The integral up to 42 meV gives a fluctuating moment of 0.8(2) μ_B.

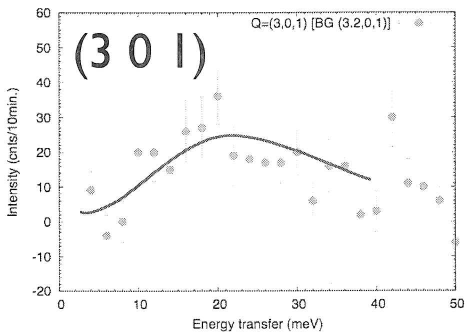
What are the characters of the scattering in the gray shaded area?

Magnetic excitations at antiferromagnetic wavevectors

Excitations were observed at (1,0,1), (1,0,3), (1,0,5), (1,0,7), and (3,0,1).

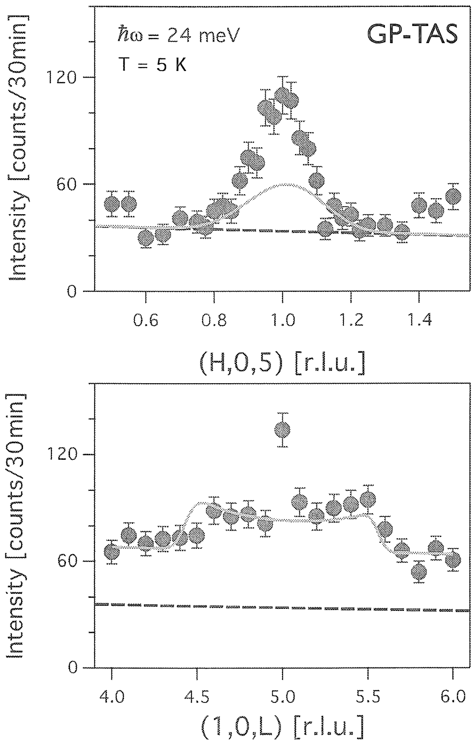






Transverse fluctuations along b-axis: Also spin-wave-like!

High energy magnetic excitations



- Yellow shaded areas : spin wave scattering

  Δ = 9.8 meV

  v_{ab} = 280 meV

  v_c = 80 meV

- Single high point is spurious.

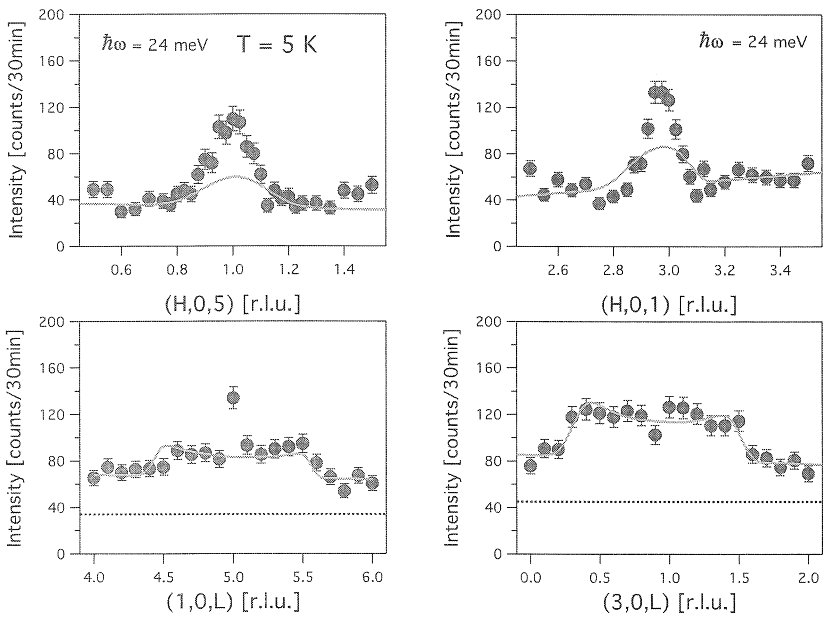
Gray shaded areas

- Also observed at (1,0,3), (3,0,1), and (1,0,7).
- Centered at the antiferromagnetic wavevectors co-existing with the spin waves.
- Anisotropic scattering indicate two-dimensional spin dynamics.

High energy magnetic excitations at 24 meV

(1 0 5)

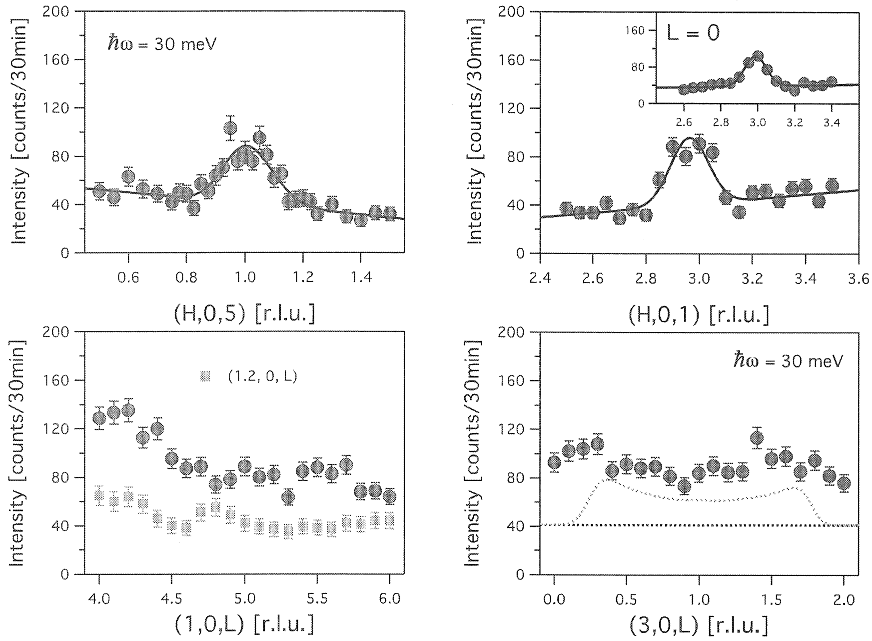
(3 0 1)



Different intensity is consistent with transverse spin waves.

High energy magnetic excitations at 30 meV

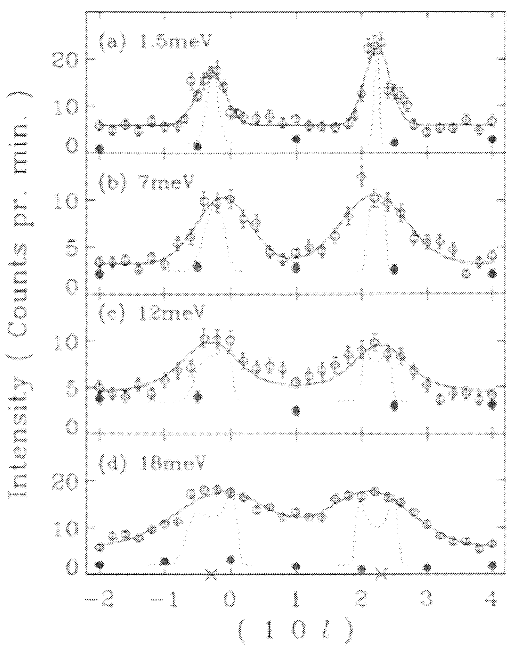
(1 0 5) (3 0 1)



What is this anisotropic scattering?

Magnetic excitations in metallic $V_{2-y}O_3$

Bao et al., Phys. Rev. B 58, 12727 (1998)

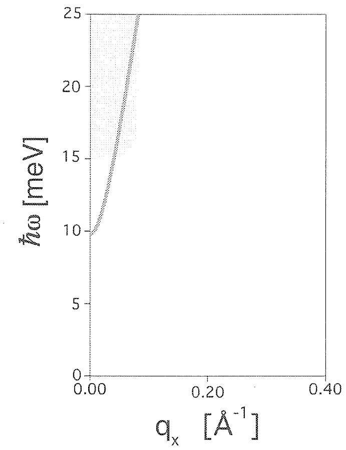


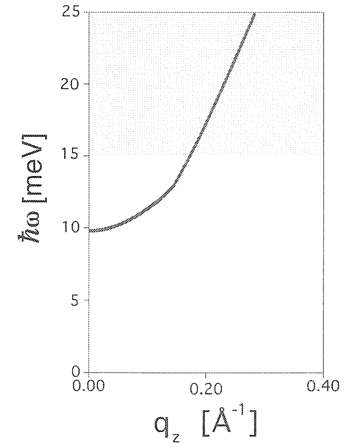
- Spins form helical ordering along the c-axis at T_N = 8.5 K with incommensurate magnetic wave vector 1.7**c***, resulting SDW instability.

Magnetic excitations

- Broad scattering that cannot be accounted for by spin waves.
- Weak coupling theory ⇒ $\hbar\omega > \Delta_s = 1.76\alpha k_B T_N$, spin wave excitations decay into the Stoner continuum.
- Δ_s = 1.4 meV is very small. Only the Stoner continuum is observed.

Presence of spin waves inside the Stoner continuum and anisotropic character are NOT reported.





Magnetic excitations in $BaFe_2As_2$

- Low energy spin wave excitations with a spin gap.
  - Also observed in $SrFe_2As_2$ and $CaFe_2As_2$.
- Anisotropic high energy magnetic excitations.
  - Possibly the Stoner electron-hole continuum?
  - NOT observed in $SrFe_2As_2$ and $CaFe_2As_2$

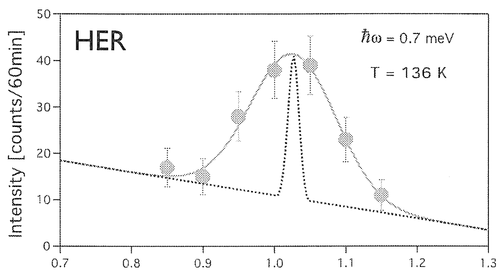
Weak coupling theory

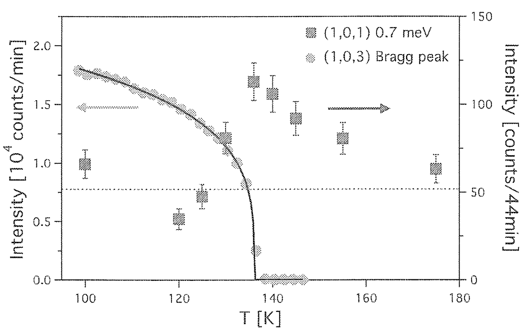
- For $BaFe_2As_2$, $\alpha \sim 1$, and $\Delta_s \sim 20$ meV.
- For $SrFe_2As_2$ (T_N = 220 K), $\Delta_s \sim 33$ meV.
- For $CaFe_2As_2$ (T_N = 172 K), $\Delta_s \sim 26$ meV.

Larger Δ_s might explain why the anisotropic scattering has not yet been observed in $SrFe_2As_2$ ($\hbar\omega_{max} \sim 16$ meV) and $CaFe_2As_2$ ($\hbar\omega_{max} \sim 25$ meV).

More experimental work is needed!

Spin fluctuations around T_N



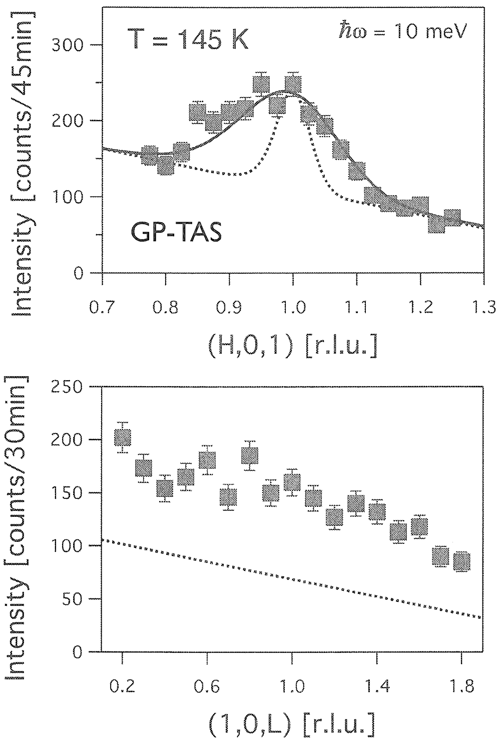


- Correlation length $\xi \sim 100$ Å ~ 40 times nearest neighbor distance.
- Temperature dependence shows a peak at T_N, coinciding with the onset of magnetic Bragg peak.
- The sharp drop on the low temperature is due to opening of the spin gap.
- The slow decrease on the high temperature side is a result of critical scattering.
- We do not observe the divergence of correlation length at T_N.

Spin fluctuations exist despite first-order magnetic transition reported in ^{75}As NMR*.

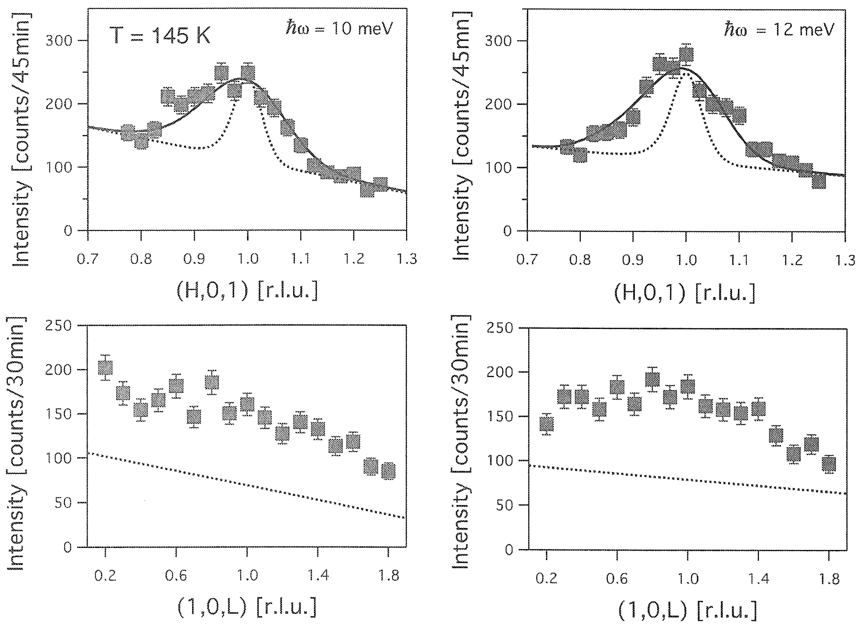
* Kitagawa et al., J. Phys. Soc. Jpn 77, 114709 (2008)

Spin fluctuations above T_N



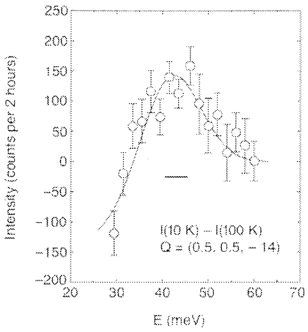
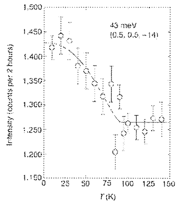
- In-plane correlation length of 80 Å or about 30 times nearest neighbor distance.
- L-scan shows "rod-like" scattering.
  - Uncorrelated interlayer spins.
- In the paramagnetic state, two-dimensional magnetism is clearly observed.
- Similar to the cuprates, large in-plane correlation length is a result of strongly two dimensional magnetism .

Spin fluctuations above T_N



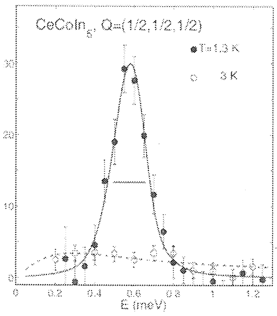
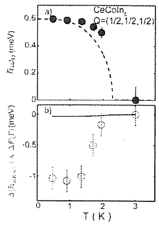
- Do spin fluctuations (enhanced by two-dimensional magnetism) remain in the superconducting state?
- Can they be responsible for superconductivity?

Magnetic excitations in superconductors

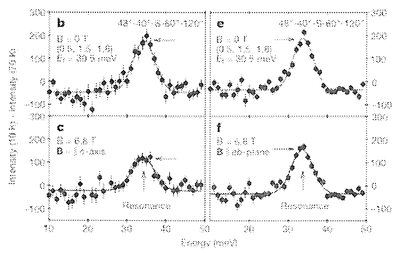
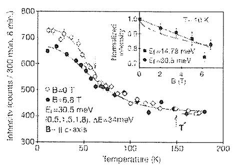
BISCCO

Fong et al., Nature 398, 588.

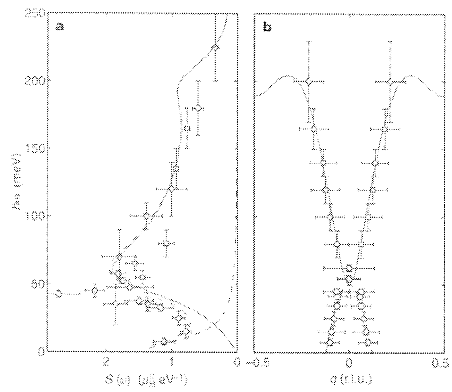
$CeCoIn_5$

Stock et al., PRL 100, 087001.

YBCO

Dai et al., Nature 406, 965.

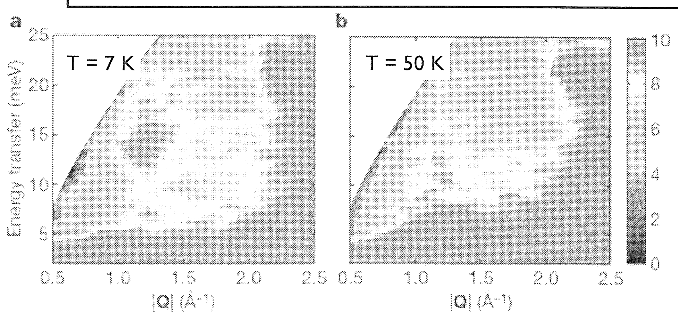
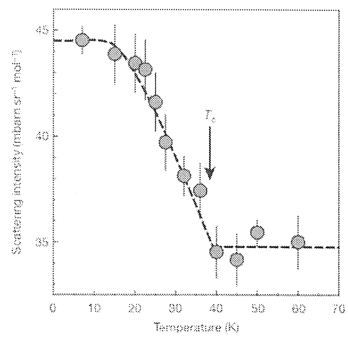


LBCO

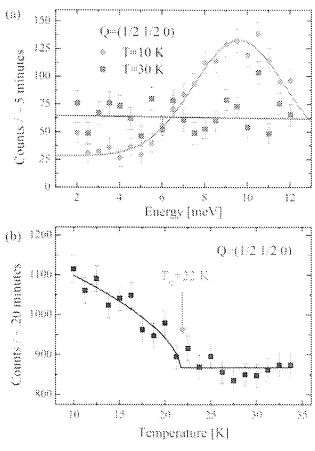
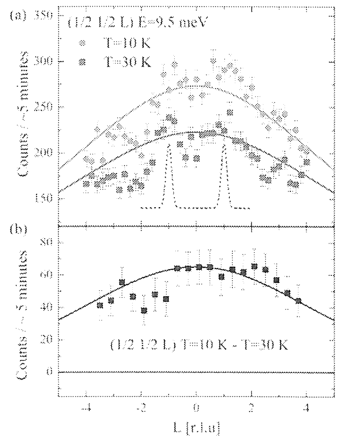
Tranquada et al., Nature 429, 534.

Magnetic excitations in superconducting state of FeAs?

Magnetic excitations in superconducting FeAs

Powdered $Ba_{0.6}K_{0.4}Fe_2As_2$ Christianson et al., Nature, 456, 930 (2008)

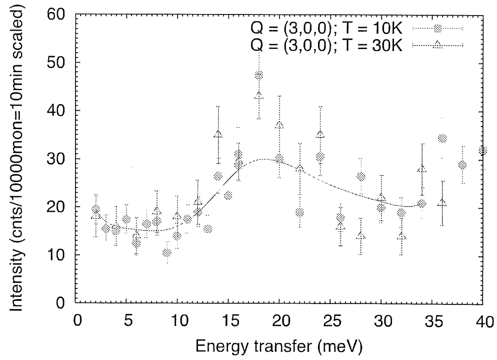
Single-crystal $BaFe_{1.84}Co_{0.16}As_2$ Lumsden et al., arXiv:0811.4755v1

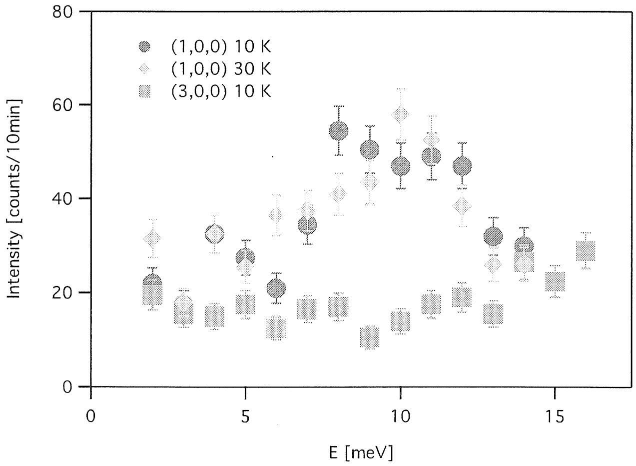
- Resonant spin excitations at 14 meV in K-doped and ~10 meV in Co-doped.
- It disappears above T_c.
- 2D nature is clearly observed.
- 2D spin dynamics are similar to high energy excitations in the ordered state, and spin fluctuations in the paramagnetic state.

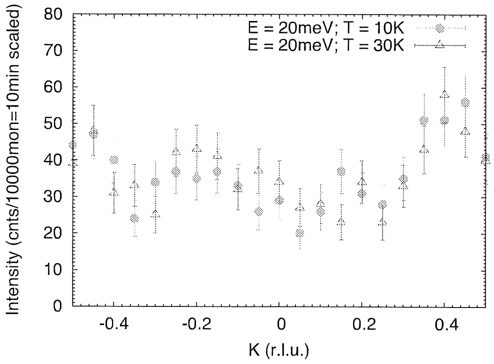
2D magnetism ⇔ superconductivity

Magnetic excitations in superconducting FeAs

- Co concentration is ~0.25-0.30 (over-doped region)
- Sample aligned in (hk0) zone







Summary

- In the ordered state, we observe low energy spin-wave-like excitations with a spin gap (origin of the gap is not clear).
- At T_N, the gap closes, and we observe spin fluctuations with large in-plane correlation length.

Goal I : Anisotropic magnetic interactions

- v_c/v_{ab} ~ 0.2 smaller than $SrFe_2As_2$ and $CaFe_2As_2$ but much larger than cuprates.
- Above T_N, we observe rod-like scattering along L, attesting the two-dimensionality of this system.

Goal II : Itinerant magnetism

- At higher energy, we observe anisotropic scattering on top of spin waves (the Stoner electron-hole continuum?).

18. Spectroscopic-Imaging STM on a $PrFeAsO_{0.7}$ Single Crystal

T. Hanaguri[1], M. Ishikado[2], S. Shamoto[2,3], H. Eisaki[3,4], A. Iyo[3,4], H. Kito[3,4] and H. Takagi[1,3,5]

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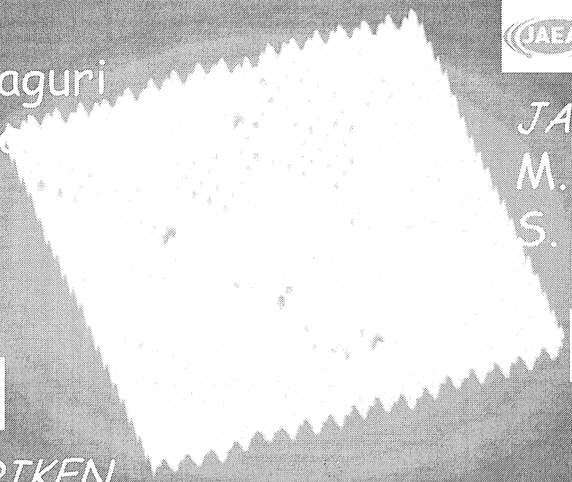
Recent developments of STM technology have enabled us to map conductance (*dI/dV*) images at various energies over wide field of view. One of the important applications of this spectroscopic-imaging STM (SI-STM) is that momentum-space electronic states can be explored through the Fourier analyses of the quasi-particle interference (QPI) patterns which appear in *dI/dV* images. In superconductors, characteristic scattering vectors for QPI contain information not only on the Fermi surface but also on the superconducting gap. QPI measurements in cuprate high-T_c superconductors have proven to be a powerful technique to determine the superconducting-gap dispersion in momentum space [1-3]. Recently, it has been shown that the phase of the superconducting gap can be highlighted in QPI patterns by introducing vortices as controllable quasi-particle scatters [2]. This effect is associated with the coherence factor of the vortex scattering and provides us with a new phase-sensitive approach for the superconducting gap [2]. In order to investigate the superconducting gap structure in an ion-oxipnictide superconductor, we have performed SI-STM on a $PrFeAs_{0.7}$ single crystal, especially paying attention to the possible $s_{\pm}$-symmetry [5]. Cleaved surface consists of two distinct atomic layers: FeAs and PrO planes. When measurement was done on the FeAs plane, clear atomic image was observed but the *dI/dV* spectrum does not show clear superconducting gap. *dI/dV* images exhibit *normal-state* QPI patterns which may be associated with the surface state. The PrO plane is rather unstable and individual atoms can not be identified in the topograph but the *dI/dV* spectrum shows clear gap structure. We discuss several implications of the observations,

References

[1] K. McElroy *et al.*, Nature **422**, 592 (2003).
[2] T. Hanaguri *et al.*, Nature Phys. **3**, 865 (2007).
[3] Y. Kohsaka *et al.*, Nature **454**, 1072 (2008).
[4] T. Hanaguri *et al.*, Science, *in press*.
[5] K. Kuroki *et al.*, Phys. Rev. Lett. **101**, 087004 (2008).

Spectroscopic-imaging STM on a $PrFeAsO_{0.7}$ single crystal



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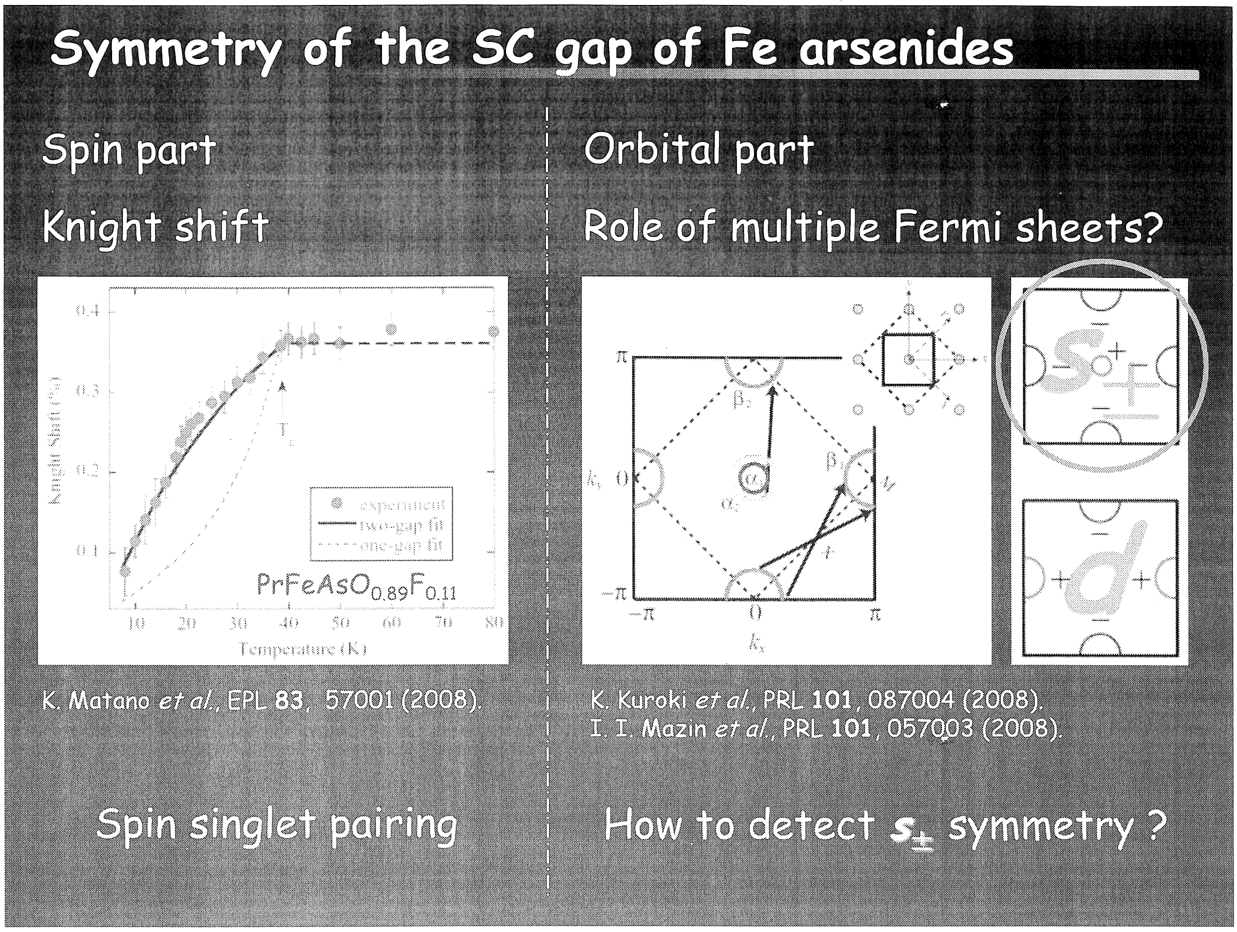
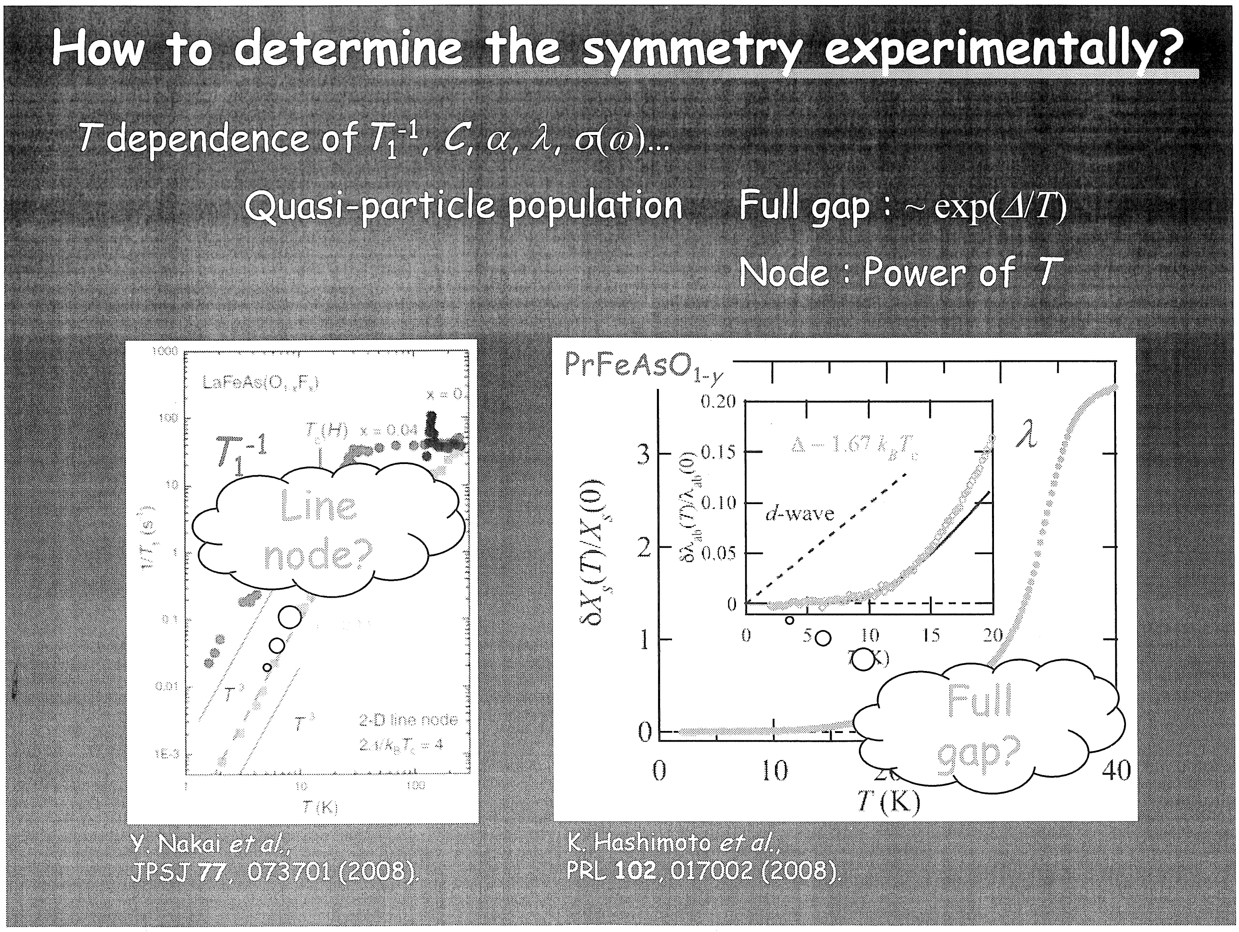
Outline

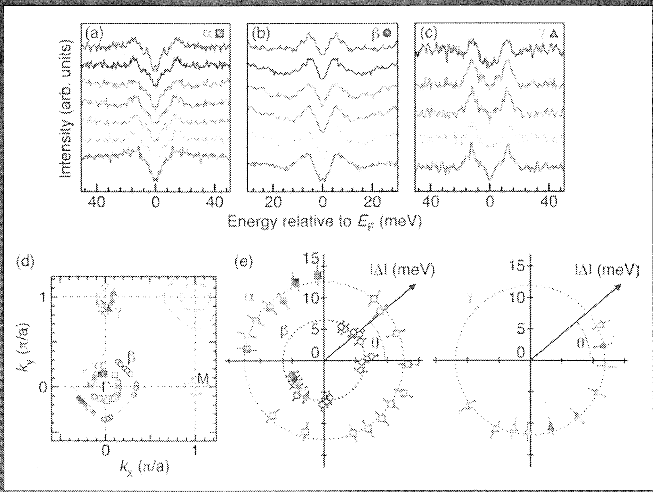
- **Motivation**
  - SC gap symmetry?
- **Why STM?**
  - Quasi-particle interference → ***k space***
  - Coherence factors → ***phase of the SC gap***
  - Case study (high-T_c cuprates)
- **Preliminary results on $PrFeAsO_{0.7}$ and Fe(Se,Te)**
  - Normal-state QPI
  - Search for SC signals
- **Summary**

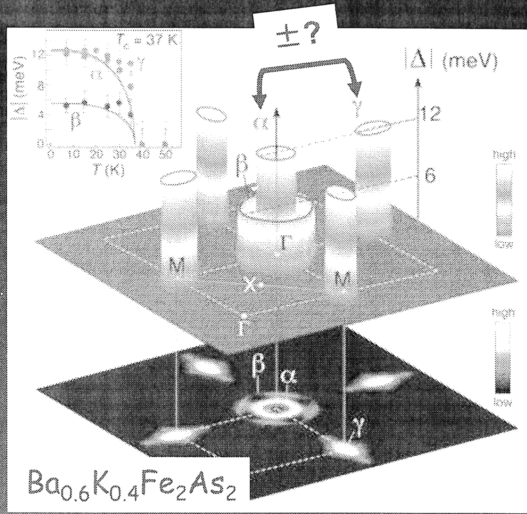

Symmetry of the SC gap of Fe arsenides
Spin part
Knight shift
Orbital part
Role of multiple Fermi sheets?
PrFeAsO0.89F0.11
Temperature (K)
Knight Shift (%)
experiment
two-gap fit
one-gap fit
K. Matano et al., EPL 83, 57001 (2008).
K. Kuroki et al., PRL 101, 087004 (2008).
I. I. Mazin et al., PRL 101, 057003 (2008).
s±
d
Spin singlet pairing
How to detect s± symmetry ?


How to determine the symmetry experimentally?
T dependence of T1-1, C, α, λ, σ(ω)...
Quasi-particle population
Full gap : ~ exp(Δ/T)
Node : Power of T
LaFeAs(O1-xFx)
T1-1
Line node?
2-D line node
T (K)
1/T1 (s-1)
PrFeAsO1-y
λ
Δ = 1.67 kBTc
d-wave
δXs(T)/Xs(0)
T (K)
Full gap?
Y. Nakai et al., JPSJ 77, 073701 (2008).
K. Hashimoto et al., PRL 102, 017002 (2008).

Direct gap map by ARPES

H. Ding *et al.*, EPL **83**, 47001 (2008)



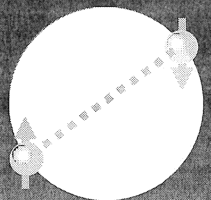


Full gap likely...

But how about the ***phase relations*** among the Fermi sheets?

Note: If $s_\pm$ symmetry, macroscopic phase-sensitive technique (e.g. π junction) does not work.

Coherence factor as a k-resolved probe



- Superconductivity : supported by Cooper pairs
- Individual QP scattering is prohibited.
- Strong coherence between $\mathbf{k}_i \rightarrow \mathbf{k}_f$ and $-\mathbf{k}_f \rightarrow -\mathbf{k}_i$

QP scattering probability

Super : $$w(i \rightarrow f) \propto |V(\mathbf{k}_i, \mathbf{k}_f)|^2 (u_{\mathbf{k}_i} u_{\mathbf{k}_f} \mp v_{\mathbf{k}_i} v_{\mathbf{k}_f})^2$$

matrix element coherence factor

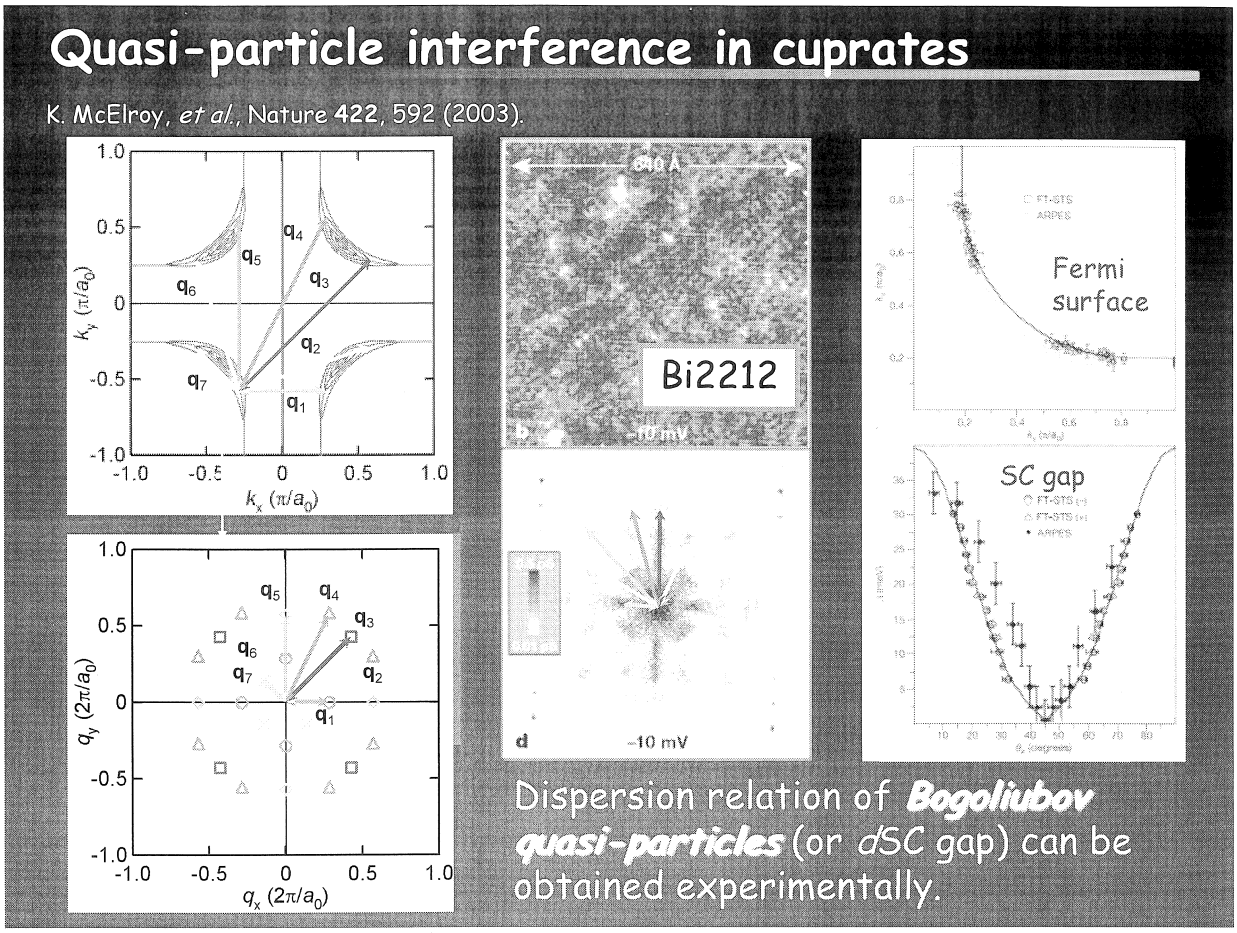
$$u_\mathbf{k} = \mathrm{sgn}(\Delta(\mathbf{k}))\sqrt{(1+\varepsilon(\mathbf{k})/E(\mathbf{k}))/2}$$

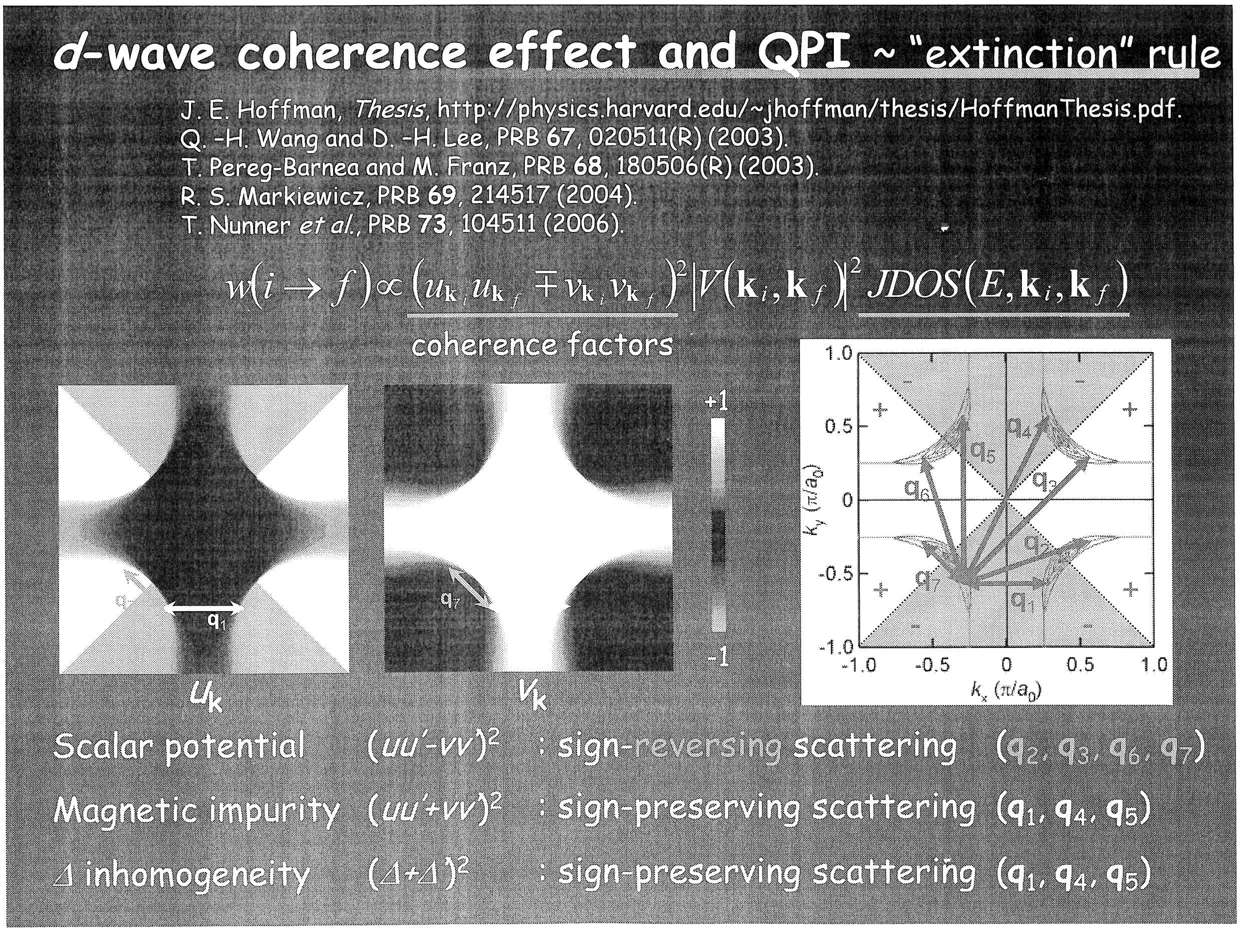
$$v_\mathbf{k} = \sqrt{1-u_\mathbf{k}^2}$$

- *s*-wave SC : *u* and *v* are isotropic.

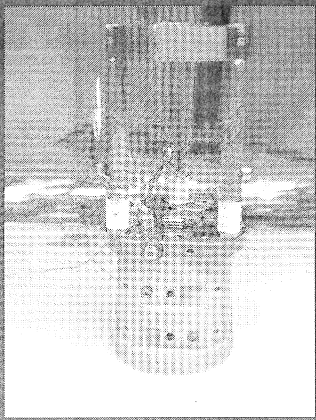
Case I (time-reversal even)	$(uu'-vv')^2$	ultrasonic etc.
Case II (time-reversal odd)	$(uu'+vv')^2$	NMR etc.

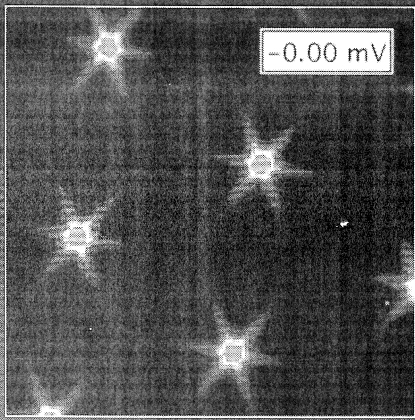
- *unconventional* SC : *u* and *v* are **k** dependent.


Quasi-particle interference in cuprates
K. McElroy, et al., Nature 422, 592 (2003).
q1 q2 q3 q4 q5 q6 q7
k_x (π/a_0)
k_y (π/a_0)
q_x ($2\pi/a_0$)
q_y ($2\pi/a_0$)
640 Å
Bi2212
-10 mV
d
Fermi surface
SC gap
Dispersion relation of Bogoliubov quasi-particles (or dSC gap) can be obtained experimentally.


d-wave coherence effect and QPI ~ "extinction" rule
J. E. Hoffman, Thesis, http://physics.harvard.edu/~jhoffman/thesis/HoffmanThesis.pdf.
Q. -H. Wang and D. -H. Lee, PRB 67, 020511(R) (2003).
T. Pereg-Barnea and M. Franz, PRB 68, 180506(R) (2003).
R. S. Markiewicz, PRB 69, 214517 (2004).
T. Nunner et al., PRB 73, 104511 (2006).
$w(i \to f) \propto \underbrace{(u_{\mathbf{k}_i} u_{\mathbf{k}_f} \mp v_{\mathbf{k}_i} v_{\mathbf{k}_f})^2}_{\text{coherence factors}} |V(\mathbf{k}_i, \mathbf{k}_f)|^2 \, \underline{JDOS(E, \mathbf{k}_i, \mathbf{k}_f)}$
+1
-1
q1
q7
$u_\mathbf{k}$
$v_\mathbf{k}$
k_x (π/a_0)
k_y (π/a_0)
Scalar potential $(uu'-vv')^2$: sign-reversing scattering (q2, q3, q6, q7)
Magnetic impurity $(uu'+vv')^2$: sign-preserving scattering (q1, q4, q5)
Δ inhomogeneity $(\Delta+\Delta')^2$: sign-preserving scattering (q1, q4, q5)

RIKEN multi-extreme STM





$NbSe_2$
T = 400 mK
H = 400 Oe
50 × 50 nm²
dI/dV map

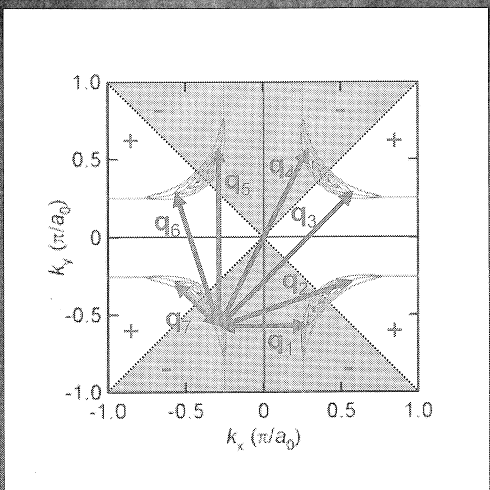
- Very-low and variable temp. (400 mK - 60 K)
- High field (11 T), UHV (~10^{-10} Torr)
- *In-situ* tip/sample exchange (resonant freq. 5.5 kHz)
- Long-term stability at base temp < Å/day
- Noise levels (2 kHz BW) < 0.5 pm, 1 pA

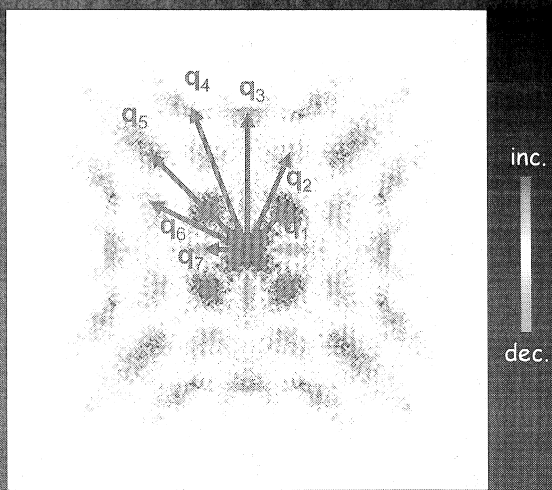
Phase-sensitive QPI in $Ca_{2-x}Na_xCuO_2Cl_2$

T. Hanaguri *et al.*, Science, *in press*. (Express Online DOI: 10.1126/science.1166138).

x ~ 0.14 V_{sample} = -0.1 V, I_t = 0.1 nA, 45nm × 45nm

FT[Z(11T)]-FT[Z(0T)]





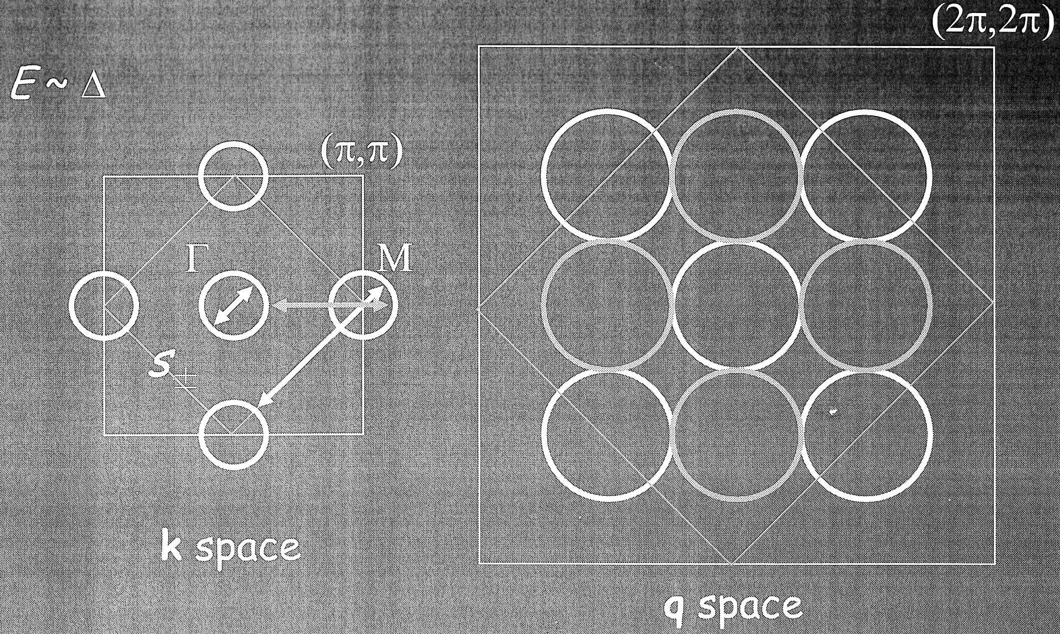
sign-preserving scattering (+,+) , (-,-) : Enhanced by B

sing-reversing scattering (+,-) , (-,+) : Suppressed by B

T. Hanaguri *et al.*, Nature Phys., **3**, 865 (2007).

Hidden ***coherence effect*** has been disclosed!!

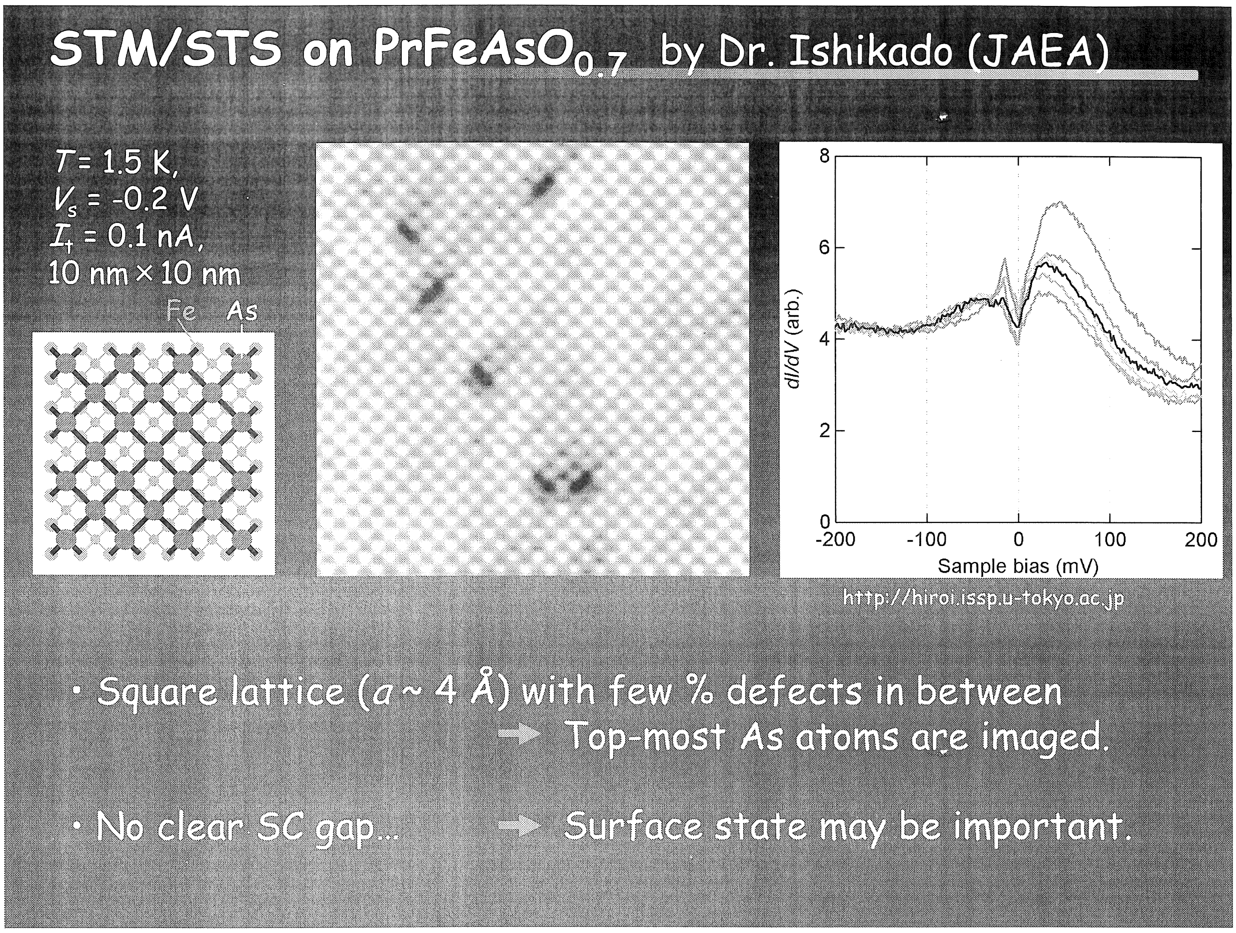
How will it work in Fe arsenides?

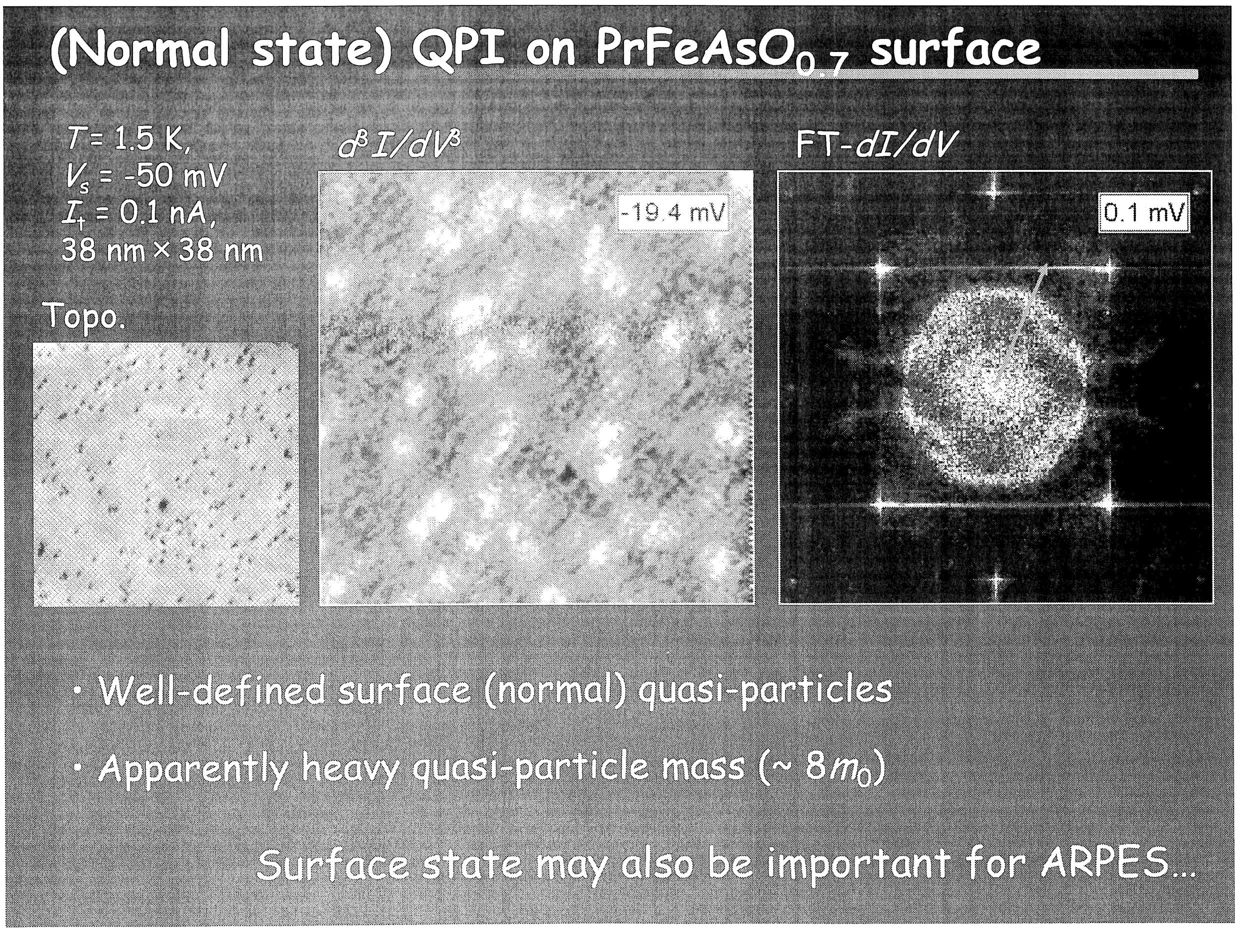


- Sign-preserving scattering
- Sign-reversing scattering

STM is a

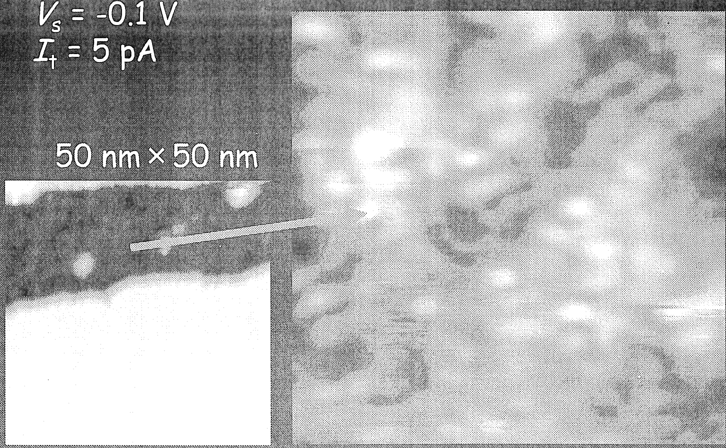
perfect experiment.

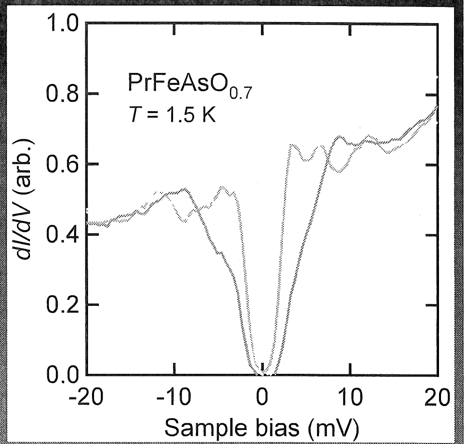

STM/STS on PrFeAsO0.7 by Dr. Ishikado (JAEA)
T = 1.5 K,
Vs = -0.2 V
It = 0.1 nA,
10 nm × 10 nm
Fe As
8
6
4
2
0
dI/dV (arb.)
-200 -100 0 100 200
Sample bias (mV)
http://hiroi.issp.u-tokyo.ac.jp
• Square lattice (a ~ 4 Å) with few % defects in between
→ Top-most As atoms are imaged.
• No clear SC gap... → Surface state may be important.


(Normal state) QPI on PrFeAsO0.7 surface
T = 1.5 K,
Vs = -50 mV
It = 0.1 nA,
38 nm × 38 nm
Topo.
d3I/dV3
-19.4 mV
FT-dI/dV
0.1 mV
• Well-defined surface (normal) quasi-particles
• Apparently heavy quasi-particle mass (~ 8m0)
Surface state may also be important for ARPES...

Search for SC signals

T = 1.5 K,
V_s = -0.1 V
I_t = 5 pA



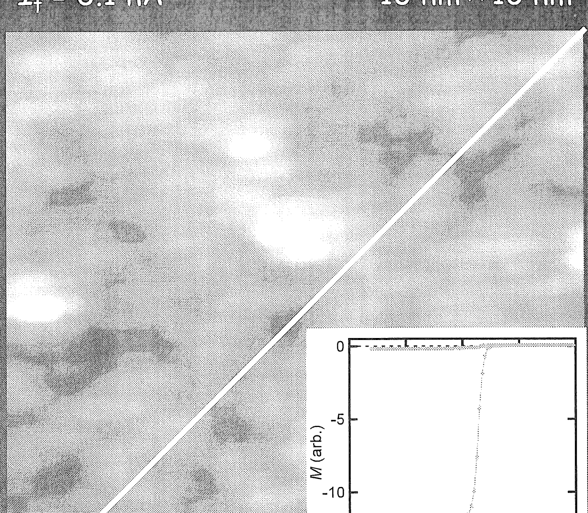


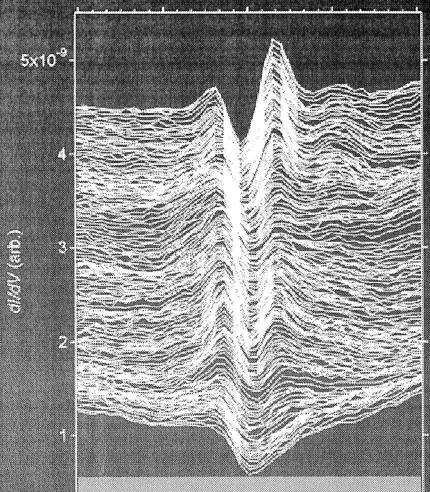
- No atomic resolution on a PrO layer (maybe)
- Apparent SC gap-like features in the spectra

More studies...

STM/STS on $Fe(Se_{0.5}Te_{0.5})$ by Dr. Niitaka (RIKEN)

T = 1.5 K,
V_s = -50 mV
I_t = 0.1 nA





Maybe SC gap but still there ia an offset at E_F...

Summary

- Quasi-particle interference patterns under magnetic fields include information on the ***phase*** of the superconducting gap. This provides us with a new method to determine the symmetry of the superconducting gap using STM.
- The top-most FeAs surface layer of cleaved $PrFeAsO_{0.7}$ does not show superconductivity but clear interference patterns of normal quasi-particles were discovered.
- The effective mass of the surface band is anomalously heavy. (~ $8m_0$)

Prospects

- Search for SC signals
  - "clean" PrO layer?
  - FeSe system (with Dr. Niitaka, RIKEN)

Fin

19. Transport and High-Pressure Study Overview

T. Ito[1,2], Y. Tomioka[1,2], N. Takeshita[1,2], R. Kumai[1,2], M. Nakajima[1,2,3], S. Ishida[1,2,3], H. Kito[1,2], K. Miyazawa[1,2], P. M. Shirage[1], H. Kihoh[1,2], M. Ishikado[2,4], A. Iyo[1,2], H. Eisaki[1,2], S. Shamoto[2,4], and S. Uchida[3]

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The iron-based superconductors are the second type of high-T_c superconductors with their maximum T_c exceeding 50 K, which is the highest besides cuprate superconductors. In order to understand the high-T_c mechanism, it is important to elucidate the similarities and differences of these two types of superconductors. In this presentation, I will compare the characteristic features of the two systems in terms of the transport properties and the pressure effects. The most characteristic feature of the iron-based superconductors is the non-linearity of the Hall resistivity with the magnetic field, which likely reflects the multiband nature of the compound [1]. The temperature- and the doping- dependence of the Hall coefficient (R_H) in the low field limit are rather small except for that in the so-called SDW phase. This is in contrast with the behavior of the cuprate superconductors, in which R_H scales with the number of doped carriers. Hydrostatic pressure dramatically affects T_c in the iron-based compounds [2], while the pressure dependence strongly depends on the materials. The behavior cannot be explained based on the simple carrier doping picture, which has been applicable in the case of the cuprate superconductors. It is more likely to be correlated with the change in the local structural parameters, such as As-Fe-As bond angle of the $FeAs_4$ tetrahedron [3]. These experimental results highlight the differences rather than similarities between the two types of high-T_c superconductors, suggesting the existence of another route to achieve high-T_c superconductivity.

References

[1] Y. Tomioka *et al.*, submitted to Phys. Rev. Lett.
[2] N. Takeshita *et al.*, J. Phys. Soc. Jpn. **77**, 075003 (2008).
[3] R. Kumai *et al.*, J. Phys. Soc. Jpn. (in press).

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Transport and High-pressure Study Overview

Toshimitsu Ito
AIST & JST
Tsukuba, Japan

Collaborators

H. Eisaki , A. Iyo, H. Kito, K. Miyazawa, P. M. Shirage (sample synthesis)

Y. Tomioka, N. Takeshita (transport)

C. H. Lee, R. Kumai, H. Matsuhata, K. Kihoh (diffraction)

M. Ishikado, S. Shamoto, M. Arai (sample synthesis, transport, diffraction)

K. Yamada, M. Braden, M.T. Fernandez-Diaz (neutron scattering)

M.Nakajima, S. Ishida, S. Uchida (transport)

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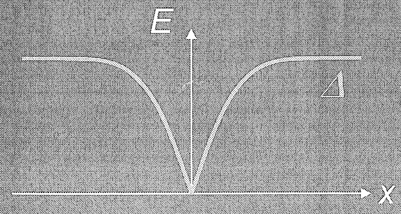
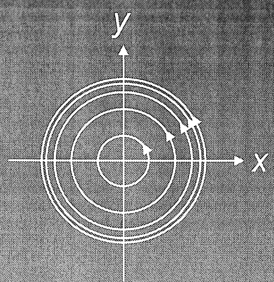
How to highlight the hidden coherence factors?

Introduce controllable QP scatterers which activate only one of the two scatterings. → ***Vortices***



Δ inhomogeneity



Phase gradient (superflow)

Δ inhomogeneity $(\Delta+\Delta')^2$: sign-preserving scattering (q_1, q_4, q_5)

Phase gradient $(uu'+vv')^2$: sign-preserving scattering (q_1, q_4, q_5)

Vortices will selectively enhance sign-preserving scatterings and highlight the ***coherence-factor effect***.

Necessary conditions for FT-QPI experiments

- k range ~ (pixel size)$^{-1}$
  > 1st BZ
  Atomic spatial resolution
- k resolution ~ (scan range)$^{-1}$
  < 1 % of BZ
  Wide field of view

Transition-metal compounds : Lattice const. ~ 4 Å

dI/dV spectra must be taken on a grid with spacing less than 2 Å over a field of view more than 400 Å × 400 Å.

256×256 points, 20 energies, 0.1 sec/energy

→ 36 hours

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Outline

1. Pressure effect

Q) What determines T_c of iron arsenide superconductors ?

- *correlation between crystal structure and T_c through artificial modification of crystal structure*

2. Transport properties

Q) What is the difference between iron arsenide and cuprate superconductors ?

- *nonlinear transport*
- *comparison of their transport properties*

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Pressure effect

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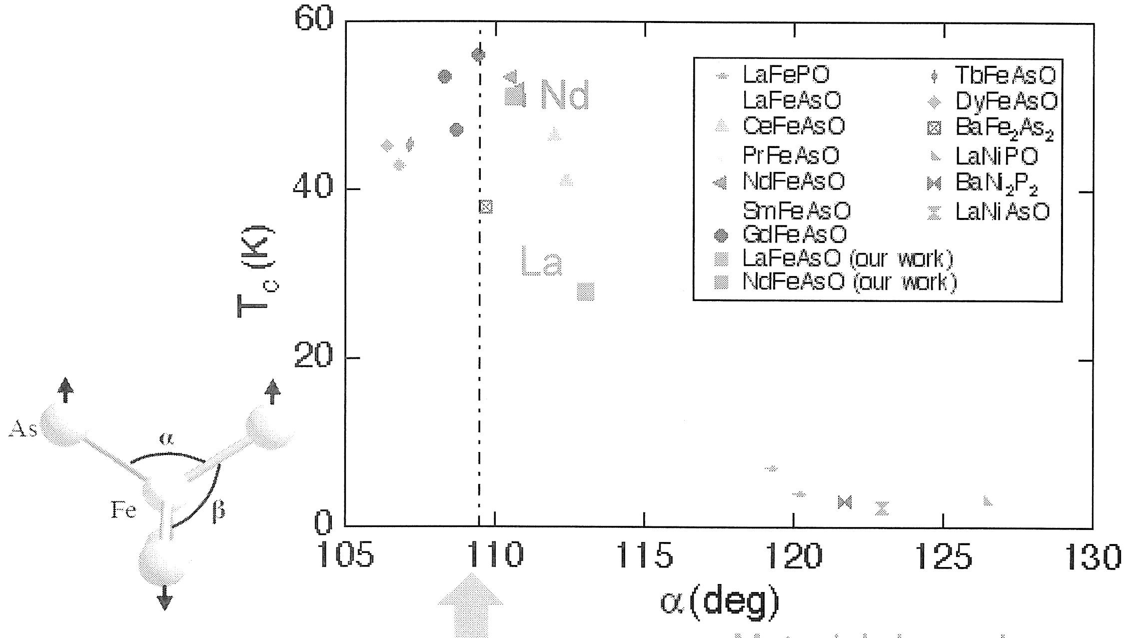
Close correlation between T_c and geometrical factor of structure



regular tetrahedron (α=β)

Material dependence

C. Lee *et al.*, JPSJ 77 (2008) 083704.

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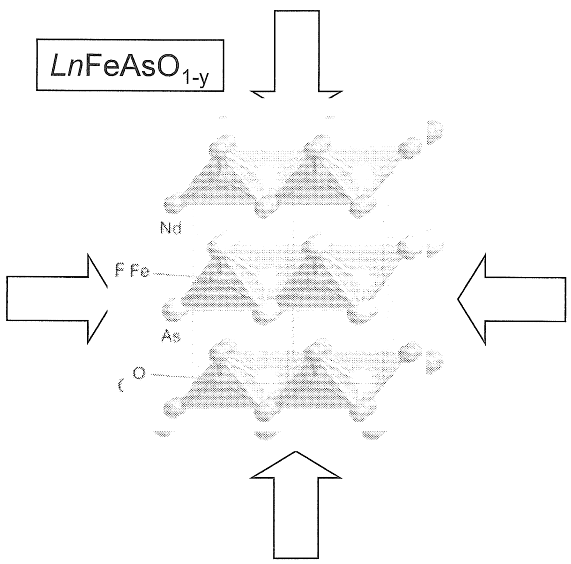
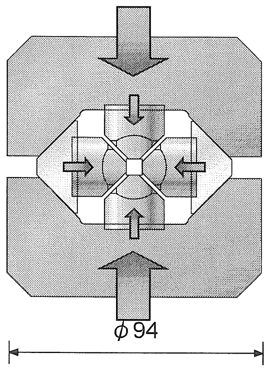
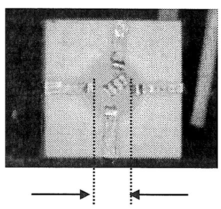
Artificial modification of crystal structure by pressure



Change in crystal structure
(lattice constant & local structure)

<u>High pressure transport</u>
(cubic anvil apparatus)





Φ2.0
Homogeneous
hydrostatic
pressure

<u>High pressure XRD</u>

·Synchrotron radiated x-ray
·Diamond anvil cell

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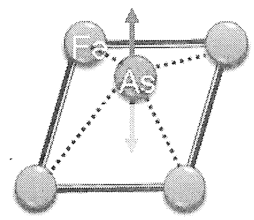
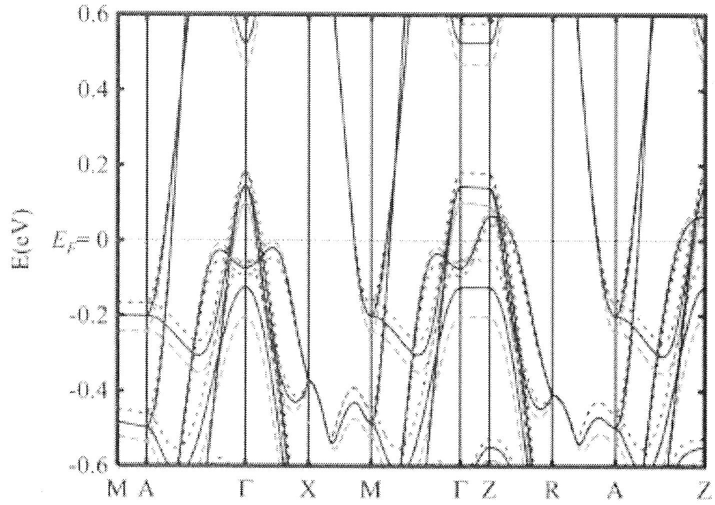
Correlation from theoretical calculations



$\delta z_{As} = 0.04$
(0.035Å)



PRL 100, 237003 (2008) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2008

Density Functional Study of $LaFeAsO_{1-x}F_x$: A Low Carrier Density Superconductor Near Itinerant Magnetism

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Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA
(Received 4 March 2008; published 12 June 2008)

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Transport Properties

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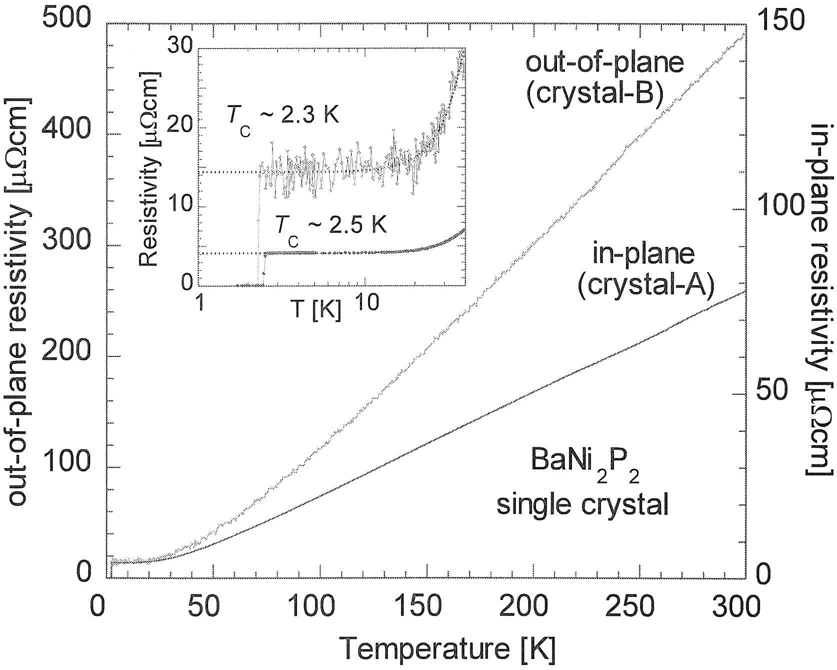
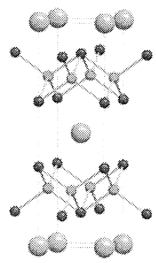
Anisotropic resistivity of $BaNi_2P_2$





$\rho_\perp/\rho_{//}$ ~ 6.3
(at 300 K)

RRR
~ 19(in-plane)
~ 35(out-of-plane)

T_C ~ 2.5 K

3D intermetallic superconductor

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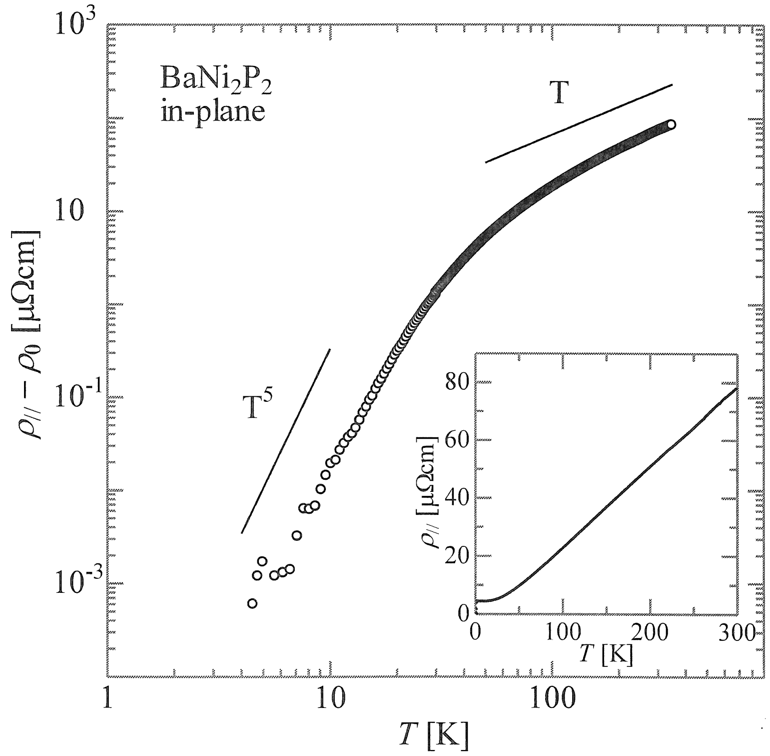
T-dependence of resistivity of $BaNi_2P_2$



Corssover
from T^5 to T

Bloch−Gruneisen

Electron−phonon
scattering

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Electron-phonon superconductivity in LaNiPO

- Low density of states of carriers
- Relatively strong electron-phonon coupling
- Tc is expected ~2.6K

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Electron-phonon superconductivity in LaNiPO

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We report first-principles calculations of the electronic structure, phonon dispersions, and electron-phonon coupling of LaNiPO. These calculations show that this material can be explained as a conventional electron-phonon superconductor in contrast to the FeAs based high-temperature superconductors.

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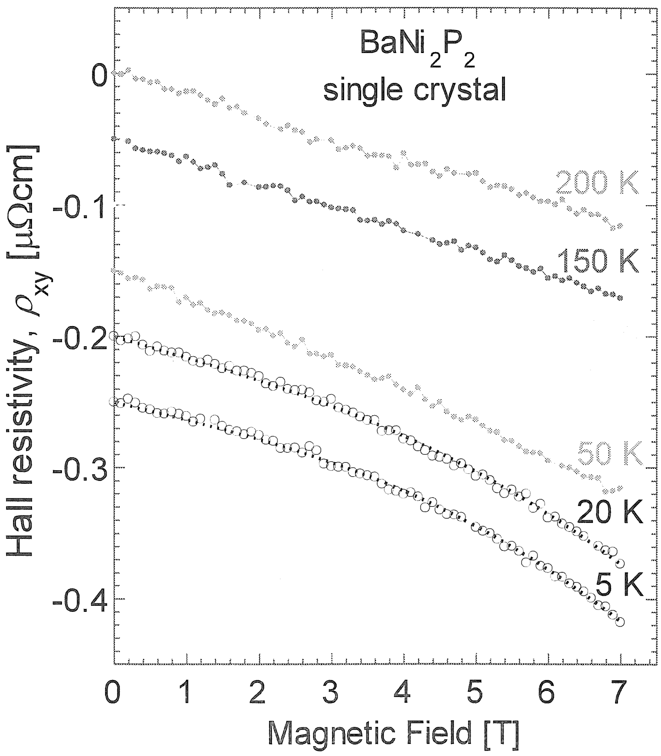
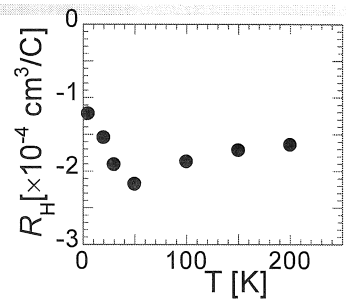
Hall resistivity of $BaNi_2P_2$





$R_H = d\rho_{xy}/dH = -1/(ne)$
$\backsim -2 \times 10^{-4}$ [cm^3/C]
($n \sim 10^{22}$ /cm^3)

Hall resistivity, ρ_{xy}
linear on H for high T
non-linear at $T < 50$ K

Multi-band

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Hall resistivity in two carrier model

"Sign reversal in the field dependence of the Hall effect in YZn…"
J.-P. Jan, N.L. Martin, and A. Wenger, Phys. Rev. B **9**, 1377 (1974).

$$\rho_{xy} = \frac{B\,[\sigma_e^2 R_e + \sigma_h^2 R_h + \sigma_e^2 \sigma_h^2 R_e R_h (R_e + R_h) B^2]}{[(\sigma_e + \sigma_h)^2 + \sigma_e^2 \sigma_h^2 (R_e + R_h)^2 B^2]}$$

(σ_e and R_e (σ_h and R_h); conductivities and Hall coefficients for electrons (holes))

$$\rho_{xy} = \frac{B\,(1/e)\,[n_h \mu_h^2 - n_e \mu_e^2 + (n_h - n_e)\mu_h^2 \mu_e^2 B^2]}{[(n_h \mu_h + n_e \mu_e)^2 + (n_h - n_e)^2 \mu_h^2 \mu_e^2 B^2]}$$

(n_e and μ_e (n_h and μ_h); carrier numbers and mobility of electrons (holes))

$(a = n_h/n_e,\ b = \mu_h/\mu_e)$

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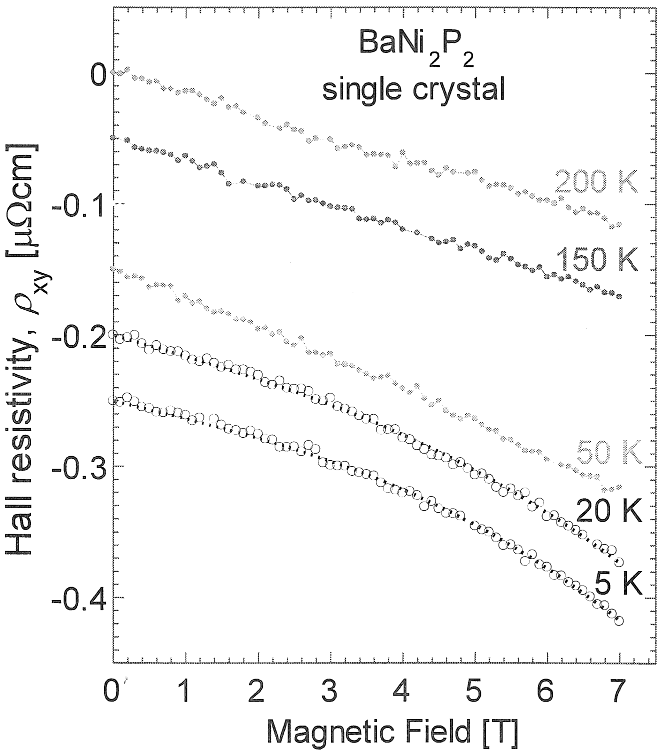
Hall resistivity of $BaNi_2P_2$



Fitting (dotted line)
$R_e = -1/(n_e e)$
$= -4.1 \times 10^{-4}$ [cm^3/C]
$\mu_e = 96$ [cm^2/Vs]
$a = n_h/n_e \sim 0.0043$
$b = \mu_h/\mu_e \sim 12.50$

Small hole FS
with high mobility

⇧

Consisitent with dHvA
T. Terashima and H. Harima

NIMS KOBE UNIVERSITY

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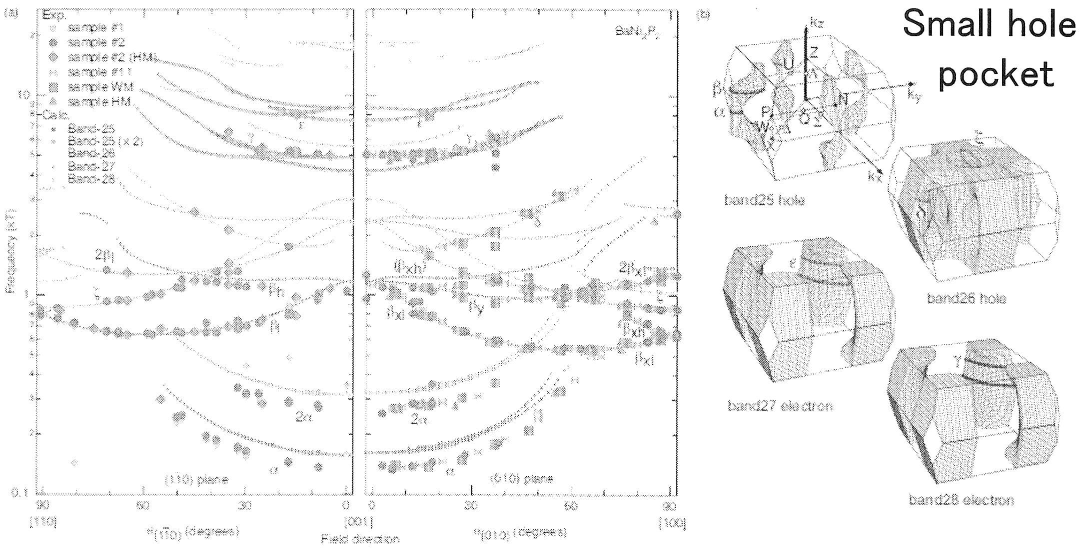
dHvA of $BaNi_2P_2$



Fermi surface in $BaNi_2P_2$ CondMat 0901.3394

Taichi TERASHIMA[1,4], Motoi KIMATA[1], Hidetaka SATSUKAWA[1], Atsushi HARADA[1], Kaori HAZAMA[1], Motoharu IMAI[1,4], Shinya UJI[1,4], Hijiri KITO[2,4], Akira IYO[2,4], Hiroshi EISAKI[2,4], and Hisatomo HARIMA[3,4]

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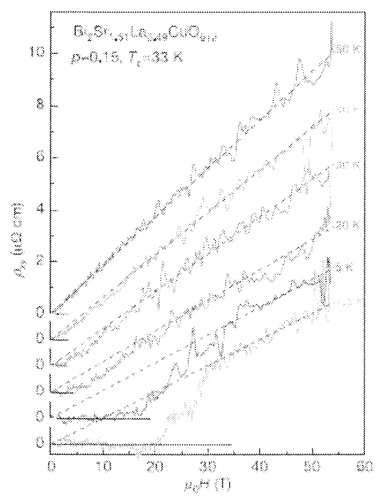
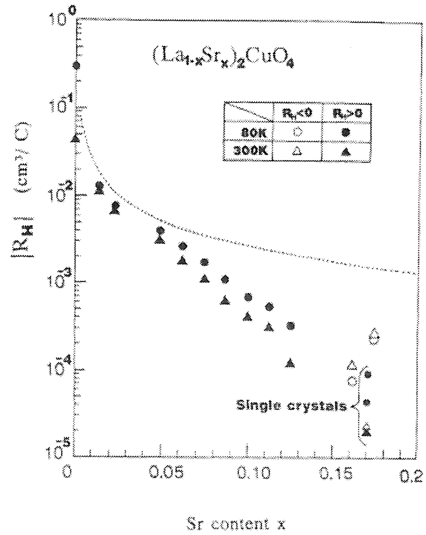
Hall coefficient of cuprate superconductors





H-linear ρ_{xy} (single band)

Doping dependence of R_H is large.

T dependence of R_H is large.

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Summary

- Possible correlation between geometrical factors in tetrahedron like bond angle and superconductivity
- Nonlinear transport due to multiband nature
- Small doping- and T-dependence of Hall coefficient in contrast to the behavior of the cuprates

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