Pnictides at high magnetic fields

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KITP, School on High-T_c superconductivity, Santa Barbara, August 12, 2009

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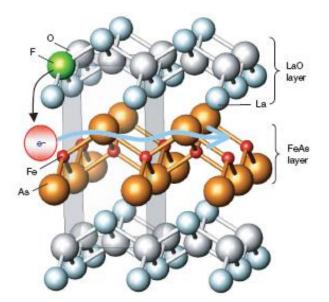
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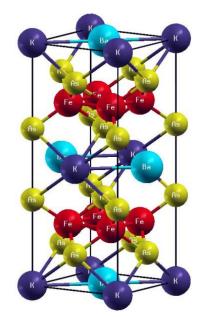
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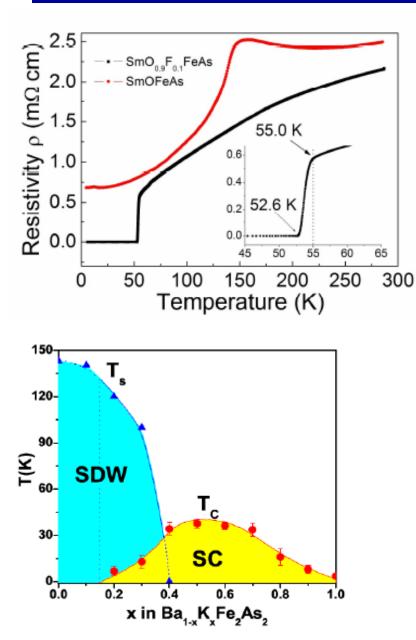
A diverse superconducting/magnetic family

- Oxypnictide base
- ReOMPn
 - M = Fe, Co, Ni
 - Pn = As or P
 - Re = La, Nd, Sm, Pr
- Superconducting AsFe layers and charge reservoir ReO layers
- Superconductivity occurs on the FeAs layer with magnetic pairbreaking Fe²⁺ ions
- Main families: ReOMPn based (1111) Ba_{1-x}K_xFe₂As₂ based (122) FeSe_xTe_{1-x} based (11)





Supercondutivity upon doping



Undopped parent compound: anisotropic semi-metal. Antiferromagnetic transition at 150K and tetragonal – orthorhombic structural transition

Becomes superconducting upon doping with F, or in the oxygen deficient form without F

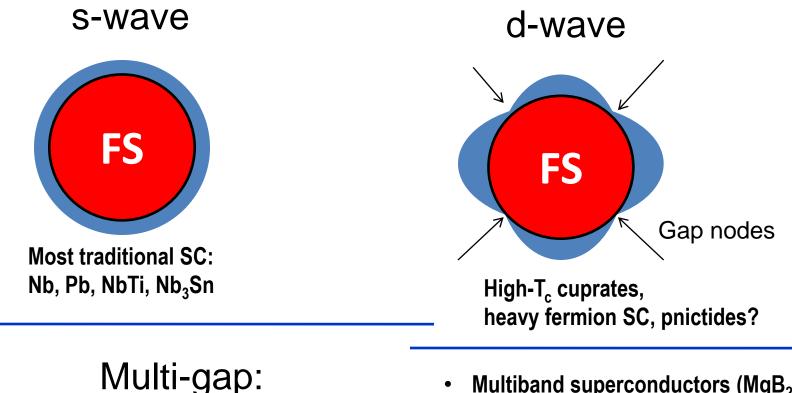
- LaO_{0.89} $F_{0.11}$ FeAs: $T_c \simeq 26K$ (43K under pressure)
- $NdO_{1-x}F_xFeAs$: $T_c \cong 52K$
- SmO_{1-x} F_x FeAs : $T_c \cong 55K$
- $PrO_{1-x}F_{x}FeAs$: $T_{c} = 52K$
- $CeO_{1-x}F_xFeAs$: $T_c = 40K$
- $Ba_{1-x}K_xFe_2As_2$: $T_c = 38K$

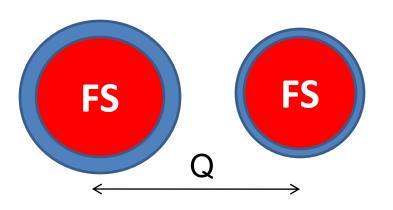
Coexistence of AF and SC

What makes oxypnictides special?

- High T_c up to 55K in a very broad family of materials (up to several hundreds compounds)
- A hope of discovering new higher-T_c pnictides and a pathway for understanding cuprates
- Superconductivity resulting from magnetic Fe ions: coexistence of superconductivity and antiferromagnetism (elemental Fe has T_c = 2K under 20 Gpa)
- Extremely high H_{c2}(0) > 100T, grossly exceeding what would be normally expected from a SC with T_c = 20-50K (well above the Pauli paramagnetic limit)
- Anomalous temperature dependence of H_{c2}(T) consistent with multiband pairing
- Small sizes of the Cooper pairs (2-3 nm): sensitivity to materials defects and strong current blocking by grain boundaries
- Competing SC/AF orders, low carrier density, strong fluctuation effects
- Rich vortex dynamics and pinning: vortex melting/vortex glass zoology + multibandband physics + interaction of vortices with magnetic structures. Some pnictides behave like HTS, some behave like LTS

Pairing gap symmetries

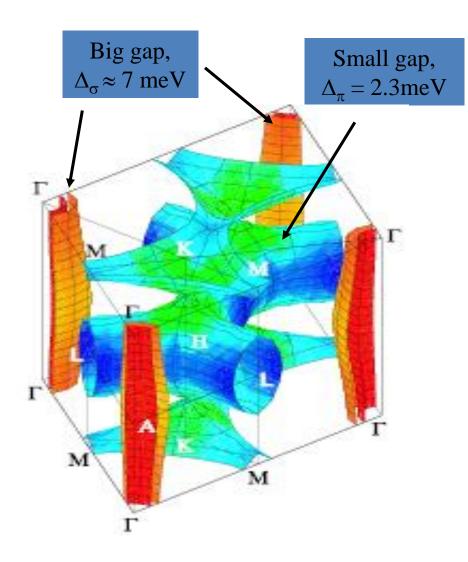


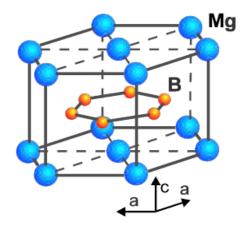


- Multiband superconductors (MgB₂, oxypnictides
- Different superconducting gaps on disconnected pieces of FS
- s-wave gaps with either same or opposite signs (s[±] pairing)
- Line nodes?

Two-gap superconductivity in MgB₂

J. Akimitsu et al, Nature 410, 63 (2001)





• 2D big gap for in-plane σ -orbitals of B and 3D small gap for out-of-plane π -orbitals of B

- Weak interband coupling
- Conventional electron-phonon pairing

Multicomponent s-wave order parameter Interband phase excitations

Critical temperature

Suhl, Mattias, Walker PRL 3, 552 (1959); Moskalenko, FMM 8, 25 (1959):

$$T_{c0} = 1.14\omega_D \exp[-(\lambda_+ - \lambda_0)/2w],$$
$$\lambda_{\pm} = \lambda_{11} \pm \lambda_{22}, \qquad \lambda_0 = \sqrt{\lambda_-^2 + 4\lambda_{12}\lambda_{21}},$$
$$w = \lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21},$$

Interband coupling increases T_c

- Weak interband pairing in MgB₂, $\lambda_{12}\lambda_{21} \ll \lambda_{11}\lambda_{22}$
- Strong interband pairing in pnictides, $\lambda_{12}\lambda_{21} > \lambda_{11}\lambda_{22}$

Pairbreaking interband impurity scattering

$$\psi\left(\frac{1}{2} + \frac{g}{t}\right) - \psi\left(\frac{1}{2}\right) = -\frac{(\lambda_0 + w\ln t)\ln t}{p + w\ln t},$$

$$2p = \lambda_0 + [\gamma_-\lambda_- - 2\lambda_{12}\gamma_{21} - 2\lambda_{21}\gamma_{12}]/\gamma_+$$

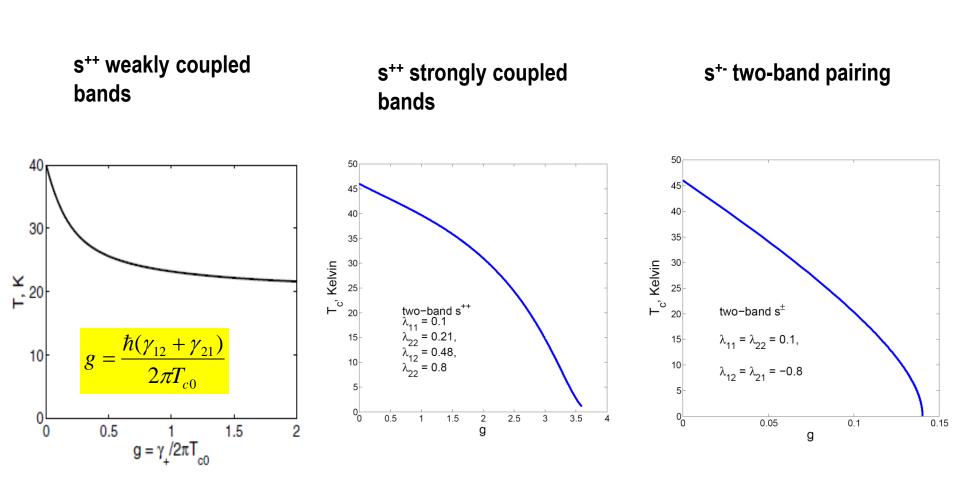
Golubov, Mazin, PRB 55, 15146 (1997); AG, PRB 67, 184515 (2003)

$$T_c \cong T_{c0} - \frac{\pi \gamma_{12}}{8} \left(1 \mp \sqrt{\frac{N_1}{N_2}} \right)^2$$

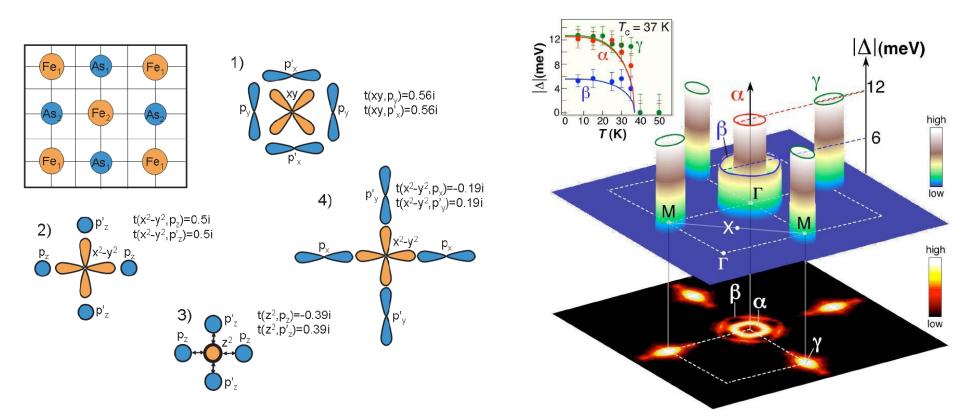
 T_c suppression is much weaker for the two-gap s⁺⁺(-) than for s[±] (+)

Effect of interband scattering on T_c

Possible scenarios



Multiband superconductivity in oxypnictides



Haule and Kotliar, NJP 025021 (2009)

Five d-orbitals of Fe hybridized with p-orbitals of As

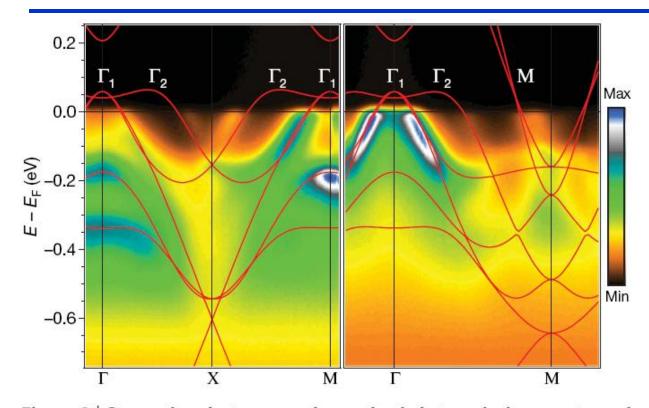
Several disconnected pieces of FS

Multiple superconducting gaps

ARPES and tunneling: Ba_{0.6}K_{0.4}Fe₂As₂

Ding et al, EL 83, 47001 (2008)

Electron spectrum from ab-initio calculations and ARPES



 multiple bands crossing the Fermi level

- qualitative consistency of ARPES and ab-initio calculations
- two hole pockets at Γ and two electron pockets at M

Figure 2 | **Comparison between angle-resolved photoemission spectra and LDA band structures along two high-symmetry lines.** ARPES data from LaOFeP (image plots) were recorded using 42.5-eV photons with an energy resolution of 16 meV and an angular resolution of 0.3°. Vol 455/4 September 2008/doi:10.1038/nature07263

TERS

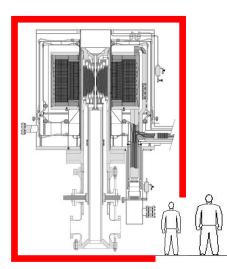
nature

Electronic structure of the iron-based superconductor LaOFeP

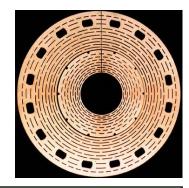
D. H. Lu¹, M. Yi¹, S.-K. Mo^{1,2}, A. S. Erickson³, J. Analytis³, J.-H. Chu³, D. J. Singh⁴, Z. Hussain², T. H. Geballe³, I. R. Fisher³ & Z.-X. Shen¹

High-field measurements at NHMFL

45T Hybrid Magnet Highest DC Magnetic Field







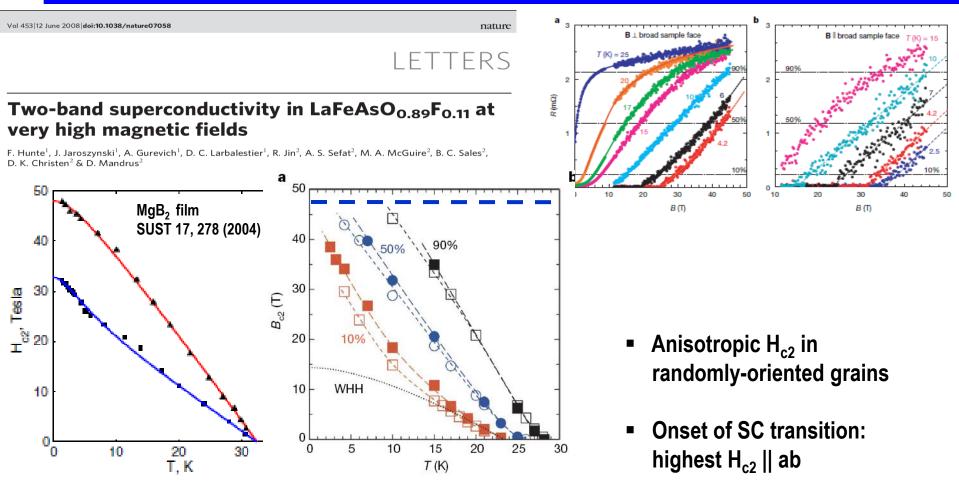
"world's highest steady-field resistive (35 T) and hybrid (45 T) magnets"

200T, 1 microsecond One pulse per hour NHMFL/LANL





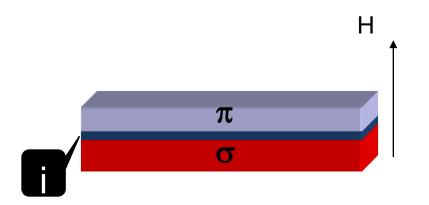
First signs of huge upper critical fields

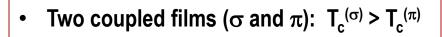


- Very high $dH_{c2}/dT = 3-10 \text{ T/K}$; extrapolation to low T suggests: $H_{c2}(0) \approx 70 \text{ T}$, well above WHH and the BCS paramagnetic limit
- Upward curvature of H_{c2}(T) for H||c, similar to MgB₂

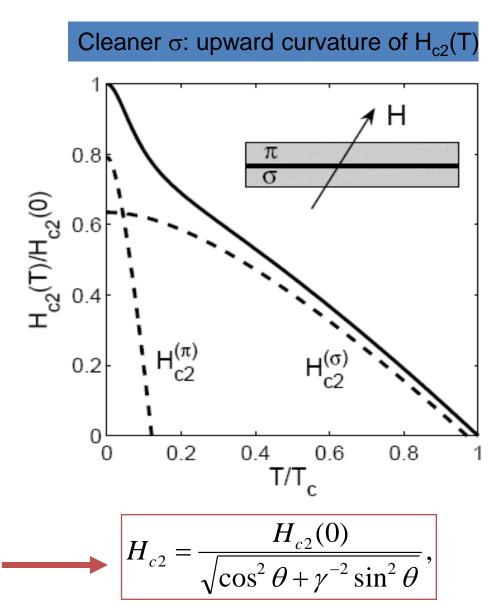
 Onset of resistivity: percolative transition for the grains with the smallest H_{c2} || c

Bilayer toy model for H_{c2} in a two-band superconductor





- Josephson interface junction mimics interband coupling
- Breakdown of the GL angular scaling: temperature dependent anisotropy
- Model-independent behavior



applied separately for each films

Two-gap superconductivity in the dirty limit

Two-gap Usadel eqs.

$$(\omega + i\mu_{B}H)f_{1} - \frac{D_{\alpha\beta}^{(1)}}{2}[g_{1}\Pi_{\alpha}\Pi_{\beta}f_{1} - f_{1}\nabla_{\alpha}\nabla_{\beta}g_{1}] = \Delta_{1}g_{1} + (f_{2}g_{1} - f_{1}g_{2})\gamma_{12}$$
$$(\omega + i\mu_{B}H)f_{2} - \frac{D_{\alpha\beta}^{(2)}}{2}[g_{2}\Pi_{\alpha}\Pi_{\beta}f_{2} - f_{2}\nabla_{\alpha}\nabla_{\beta}g_{2}] = \Delta_{2}g_{1} + (f_{1}g_{2} - f_{2}g_{1})\gamma_{21}$$

Here $D_{\alpha\beta}$ are intraband electron diffusivities, $\Pi = \nabla + 2\pi i A/\phi_0$, γ are interband scattering rates, λ_{nm} is 2×2 matrix of BCS coupling constants.

• Gap equations:

$$\Delta_{\mathbf{m}} = 2\pi T \sum_{\omega>0}^{\omega_{\mathbf{D}}} \sum_{s=1,2} \lambda_{\mathbf{m}s} \mathbf{f}_{s}(\omega, \Delta_{s})$$

Equation for H_{c2} including inter and intraband scattering, and paramagnetic effects in the dirty limit

AG, PRB 67, 184515 (2003); Physica C546, 160 (2007)

$$2\mathbf{w}\mathbf{F}_{+}\mathbf{F}_{-} + (\lambda_{0} + \tilde{\lambda})\mathbf{F}_{+} + (\lambda_{0} - \tilde{\lambda})\mathbf{F}_{-} = \mathbf{0},$$
$$\mathbf{F}_{\pm} = \ln t + \operatorname{Re}\psi\left(\frac{1}{2} + \frac{\Omega_{\pm} + i\mu_{B}\mathbf{H}}{2\pi T}\right) - \psi\left(\frac{1}{2}\right),$$

$$2\Omega_{\pm} = \omega_{+} + \gamma_{+} \pm \sqrt{\omega_{-}^{2} + \gamma_{+}^{2} + 2\gamma_{-}\omega_{-}},$$
$$\gamma_{\pm} = \gamma_{12} \pm \gamma_{21}, \qquad \omega_{\pm} = (\mathbf{D}_{1} \pm \mathbf{D}_{2})\pi \mathbf{H} / \phi_{0},$$

$$\widetilde{\lambda} = \left[(\omega_{-} + \gamma_{-})\lambda_{-} - 2\lambda_{12}\gamma_{21} - 2\lambda_{21}\gamma_{12} \right] / \Omega_0$$

- Can be used for different pairing mechanisms
- Application to MgB₂: weak interband pairing: λ₁₂λ₂₁ << λ₁₁λ₂₂
- Application to pnictides: strong interband pairing: λ₁₂λ₂₁ > λ₁₁λ₂₂

Nd-1111 single crystal

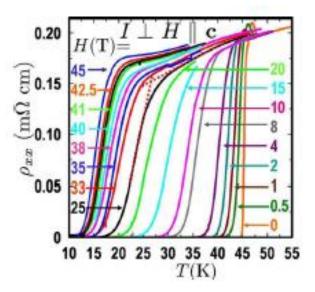
Upper critical fields and thermally-activated transport of NdFeAsO_{0.7}F_{0.3} single crystal

J. Jaroszynski, F. Hunte, L. Balicas, Youn-jung Jo, I. Raičević, A. Gurevich, and D. C. Larbalestier National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA

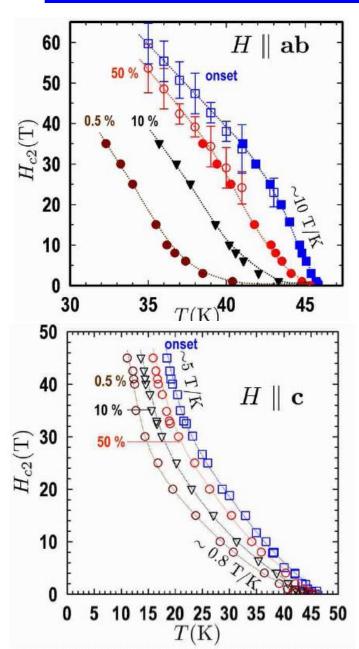
F. F. Balakirev

National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

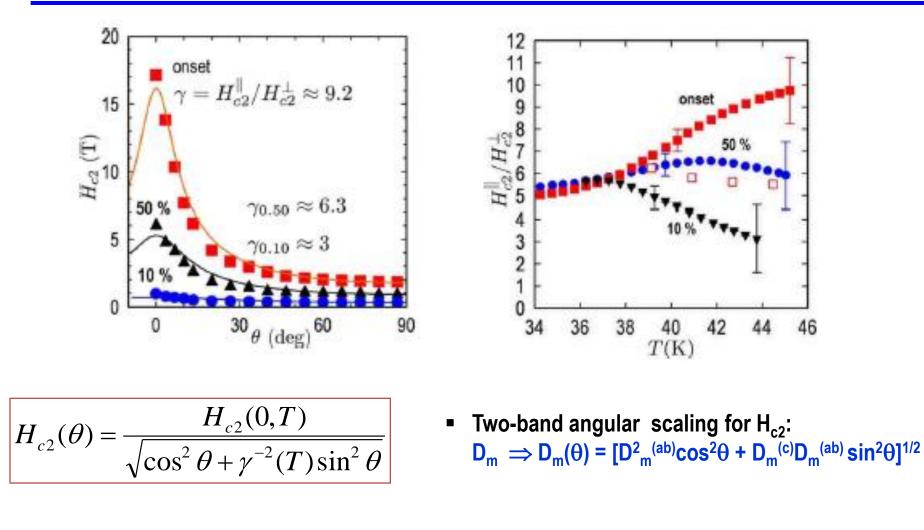
L. Fang, P. Cheng, Y. Jia, and H. H. Wen Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of China (Received 14 October 2008; published 21 November 2008)



- Combined dc (Tallahassee) and pulse (LANL) fields
- The same multiband behavior of H_{c2}(T) as on La-1111 polycrystals
- Naïve extrapolation to T=0 suggests H_{c2} ||ab \approx 200-300 T



Nd-1111 single crystals: temperature-dependent anisotropy



- GL single-band scaling is not too bad
- Temperature-dependent $\gamma(T)$ indicates multiband superconductivity
- Different dependencies of $\gamma(T)$ for H_{c2} (onset) and irreversibility field (10%)

Nd-1111 single crystals: clean or dirty?

• GL coherence lengths $\xi_{ab}(0)$ and $\xi_c(0)$ estimated from the observed $H_{c2}(T)$ slopes near T_c :

$$\xi_{ab} = \left(\frac{\phi_0}{2\pi T_c |H_{c2}|}\right)^{1/2} \cong 2 - 3nm, \qquad \xi_c = \frac{\xi_{ab}}{\gamma} \cong 0.3 - 0.4nm$$

for
$$H_{c2}^{\prime} = 2-4$$
 T/K, $\gamma = 7-10$

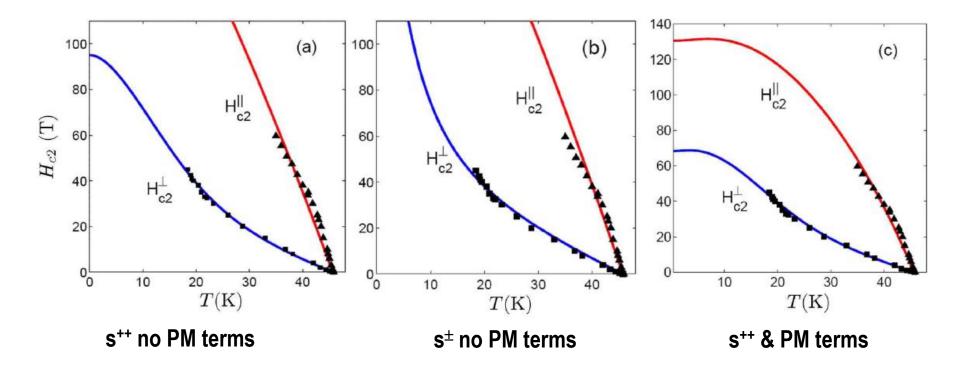
- the numbers are similar to those for YBCO
- Drude mean-free path estimated from ρ_n(T_c):

$$\ell = \frac{m^* v_F}{\rho_n n e^2} = \frac{\lambda_L^2 v_F \mu_0}{\rho_n} \cong 2 - 3nm$$

$$\label{eq:rho_n} \begin{split} \rho_n(T_c) &\approx 0.2\text{-}0.3 \ \text{m}\Omega\text{cm}, \ \lambda_L \approx 200 \ \text{nm}, \\ v_F &= 1.3^*10^7 \ \text{cm/s} \end{split}$$

- Moderately dirty limit, $\xi_{ab}(0) \approx \ell$.
- Dirty limit is applicable
- Unclear what part of $\rho_n(T_c)$ comes from nonmagnetic impurity scattering

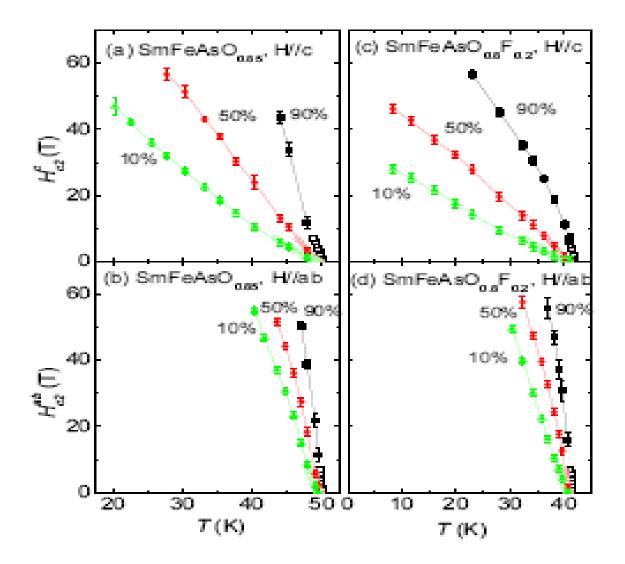
Two-band analysis of H_{c2} in Nd-1111 single crystal



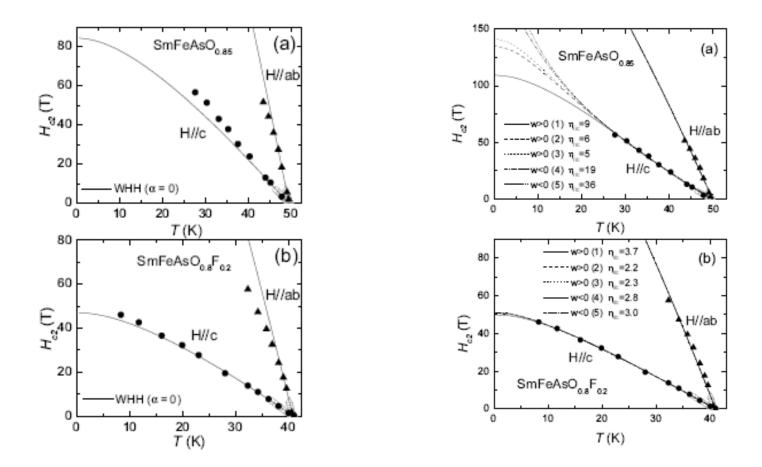
- Reproducing the observed upward curvature of H_{c2}(T) requires a significant difference in the band diffusivities D₁ and D₂
- s^{++} two-band pairing: $D_2 \approx 0.1D_1$ (a)
- s[±] pairing requires $D_2 \approx 0.01D_1$ (b)
- Pauli pairbreaking reduces the extrapolated $H_{c2}(0)$ from 200-300 T down to 60-120T

60 T pulse measurements on Sm-1111 crystals

H.-S. Lee et al, arXiv: 0908.1287

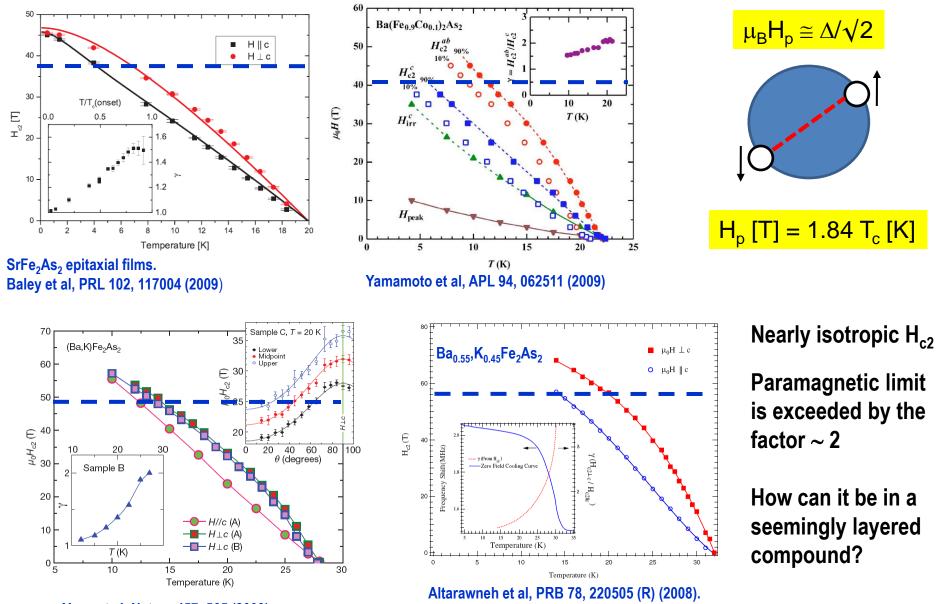


Single band versus multiband analysis



60 T is not enough to distinguish between different scenarios

PM limit in pnictides is greatly exceeded



Yuan et al, Nature 457, 565 (2009)

Paramagnetic limitations of H_{c2}

BCS one-gap paramagnetic limit (Chandrasekhar; Klogston (1962); Maki (1964));

$$\mu_{\rm B} \mathbf{H}_{\rm p} = \Delta / \sqrt{2} \qquad \Longrightarrow \qquad B_p[T] = 1.84T_c[K]$$

- Which gap in multiband superconductors?
- For T = g = 0, both D_{σ} and D_{π} should be replaced by effective diffusivities

$$\widetilde{\mathbf{D}}_{\sigma} = \sqrt{\mathbf{D}_{\sigma}^2 + \mathbf{D}_0^2}, \qquad \qquad \widetilde{\mathbf{D}}_{\pi} = \sqrt{\mathbf{D}_{\pi}^2 + \mathbf{D}_0^2}$$

• Quantum diffusivity:

$$\mathbf{D}_0 = \hbar / 2\mathbf{m}$$

(diffusion relation and the energy uncertainty principle $L^2 = Dt$ and $\hbar/t = \hbar^2/2mL^2$)

How dirty should it be to reach the PM limit?

- Impurity diffusivity = quantum diffusivity: $\frac{1}{V_F}/3 = \frac{\hbar}{2m}$
- Fermi-Compton mean free path:



For $v_F \sim 10^7 - 10^8$ cm/s (depending on the orientation), we get $\ell \sim 2 - 20$ Å

Easier to reach in pnictides because of their small Fermi velocities $v_F \cong 10^7 \mbox{ cm/s}$

PM limit in two-gap superconductors

• Maximum possible field H_p in the extreme dirty limit $D_1 \ll D_0$ and $D_2 \ll D_0$:

$$\mathbf{H}_{p}^{(max)} = \frac{\pi T_{c}}{2\gamma \mu_{B}}$$

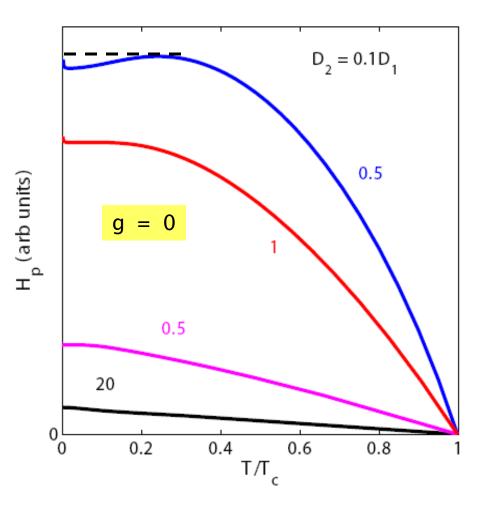
Same as in one-gap SC

• Two more limiting cases:

$$\mathbf{H}_{p} = \frac{\pi T_{c}}{2\gamma \mu_{B}} \exp\left(-\frac{\lambda_{-} + \lambda_{0}}{2w}\right) << \mathbf{H}_{p}^{(max)}, \qquad \mathbf{D}_{0} << \mathbf{D}_{1} \exp(-\lambda_{0} / w) \qquad \text{(dirty 2)}$$

$$\mathbf{H}_{p} = \frac{\pi T_{c}}{2\gamma \mu_{B}} \exp\left(\frac{\lambda_{-} - \lambda_{0}}{2w}\right) \approx \mathbf{H}_{p}^{(max)}, \qquad \mathbf{D}_{0} << \mathbf{D}_{2} \exp(-\lambda_{0} / w) \qquad \text{(dirty 1)}$$

PM first order phase transition induced by strong disorder

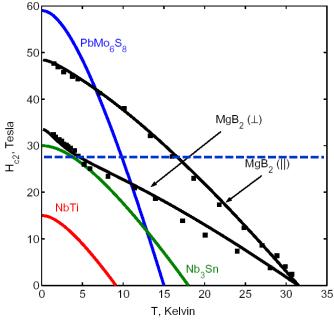


Nonmonotonic $H_p(T)$ for small values of the control parameter D_{σ}/D_0

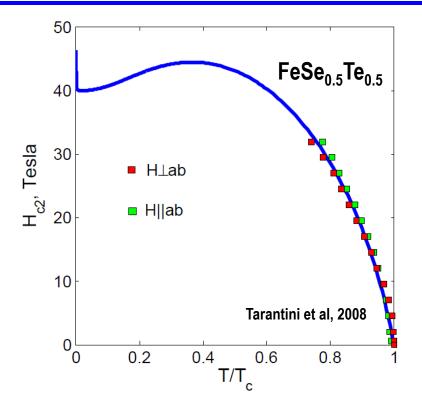
First order phase transition between N and S state at low T

Similar to the paramagnetic first order transition in the one-gap BCS theory (Sarma, 1963, Maki, 1964)

Crossover from orbital to paramagnetically limited H_{c2}



- Pnictides are not exceptional: for PbMo₆S₈ H_{c2}(0) > 2H_p^{BCS}
- Enhancement of H_p by spin-orbit interaction and strong coupling effects

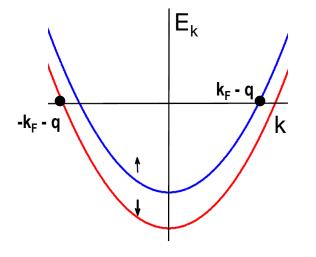


 Quasi-isotropic H_{c2}(T) might reflect the crossover from anisotropic orbital to isotropic Pauli pairbreaking

Werthammer, Helfand, Hohenberg, Phys. Rev. 147, 291 (1966) Orlando, McNiff, Foner, Beasley, PRB 19, 4545 (1979) Schlossman, Carbotte, PRB 39, 4210 (1989)

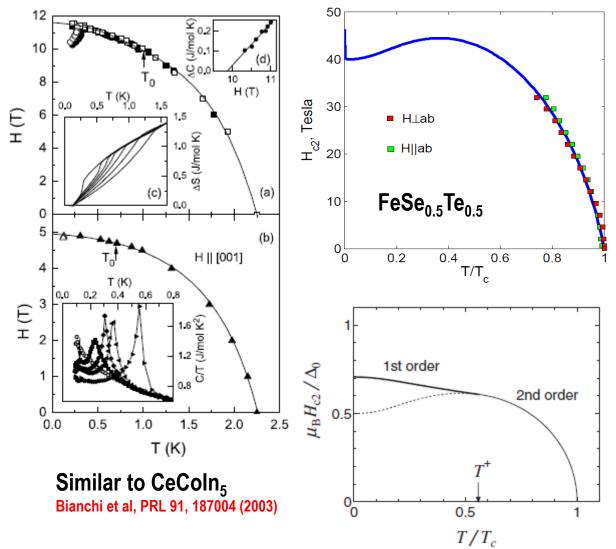
$$H_p = (1 + \lambda) H_p^{BCS}$$

Can FFLO state occur in pnictides?



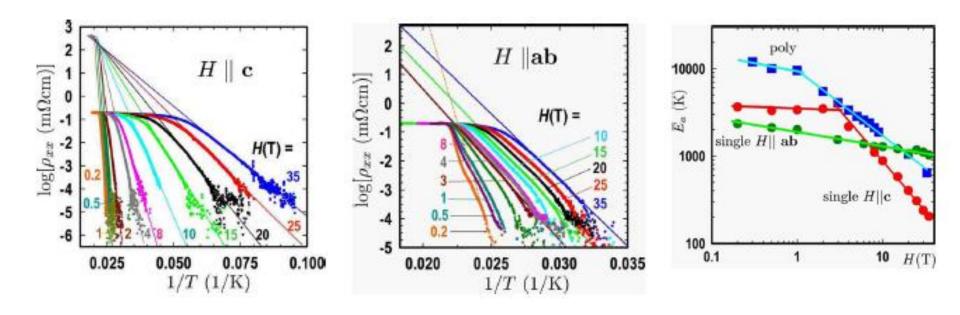
Paramagnetic depairing: in-plane modulation of the order parameter for H||ab

 $\Delta(\mathbf{x}) = \Delta_0 \cos(2q\mathbf{x})$



FFLO in pnictides requires very high fields

Nd-1111 single crystal: thermally-activated vortex dynamics



 Thermally-activated TAFF resistivity over 4-5 decades in ρ:

$$\rho = \rho_0 \exp[-E_a(T,B)/T]$$

$$E_{a} = \frac{E_{0}(1 - T/T_{c})^{\alpha}}{\left[1 + B/B_{0}(T)\right]^{\beta}} \left[1 - \frac{B}{B_{c2}(T)}\right]^{\beta}$$

• $E_0 \sim 10^2 - 10^3$ K, $B_0 \cong 3T$, $\alpha \approx 1$, and $\beta = 1.1$, B||c, and $\beta = 0.17$ B||ab Similar to YBCO J. Jaroszynski et al, PRB 78, 174523 (2008)

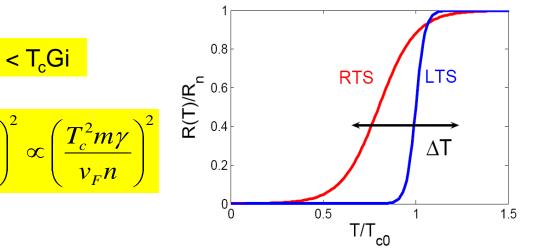
Strong thermal fluctuations in 1111-pnictides

- Critical fluctuation region: $\Delta T = T_c T < T_c Gi$
- Ginzburg parameter: $Gi = \frac{\gamma^2}{2} \left(\frac{k_B T_c}{H^2 \xi^3}\right)^2 \propto \left(\frac{T_c^2 m \gamma}{v_c n}\right)^2$

• Anisotropy parameter and the London penetration depth in a uniaxial superconductor:

$$\gamma = \left(\frac{m_c}{m_{ab}}\right)^{1/2} = \frac{\lambda_c}{\lambda} = \frac{\xi}{\xi_c} \qquad \qquad \lambda = \left(\frac{mc^2}{4\pi e^2 n_s}\right)^{1/2} \qquad \Delta T_c \propto T_c^5 \gamma^2 / n^3$$

- LTS: Gi ~ 10⁻⁸, ΔT ~ 10⁻⁷ K
- YBCO: Gi ~ 0.1-10⁻², ΔT ~ 1-10 K
- 122 pnictides: Gi ~ 10⁻⁴ -10⁻³
- 1111 pnictides: **Gi** ~ 10⁻²
- T_c reduction by phase fluctuations
- Melting of the vortex lattice. Reduced irreversibility field, H*(T) < H_{c2}(T). Numerous vortex glasses



Melting of the vortex lattice

 Lindemann criterion: (Nelson et al; Hougtion, Pelcovits, Sudbo; Blatter et al, Brandt et al)

 $\langle u^2 \rangle$ = c_L² ϕ_0/B , c_L \approx 0.15-0.17

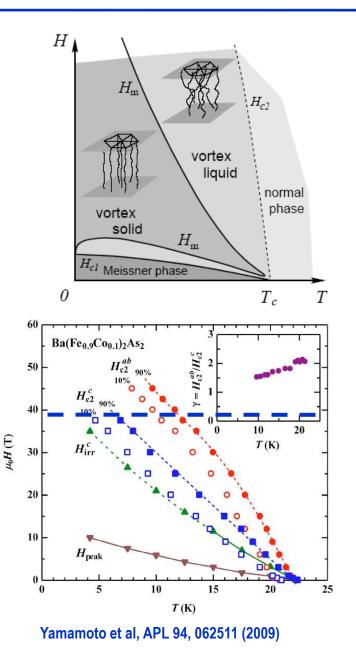
Upper branch of the melting field B_{c1} << B_m << B_{c2}:

$$\frac{B_m}{B_{c2}(0)} \approx \alpha \left(1 - \frac{T_c}{T}\right)^2, \qquad \alpha = \frac{\pi^2 c_L^4}{Gi}$$

- For Nd-1111, $\gamma = 7$, Gi = 0.01, c_L = 0.15, $\kappa = \lambda/\xi \sim 10^2$ we get $\alpha \approx 0.5$
- Low carrier density and strong anisotropy in Nd-1111 reduce the melting field well below H_{c2}

$$B_m \propto rac{1}{\gamma^2 \lambda_L^4 T_c^2}$$

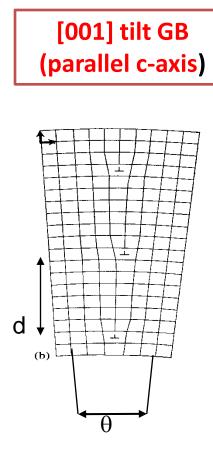
• Effect of thermal fluctuations is much weaker in 122



Types of grain boundaries

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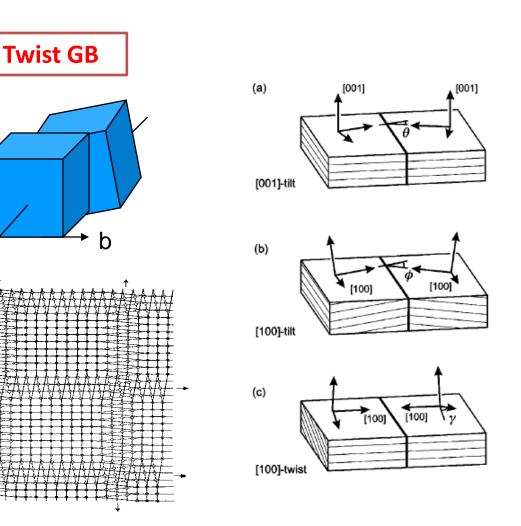
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Chain of edge dislocations spaced by

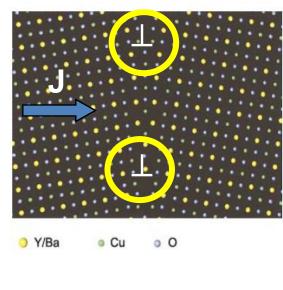
 $d = b/2sin(\theta/2)$

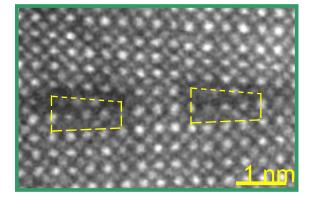
Cellular structure of twist dislocations in the ab plane



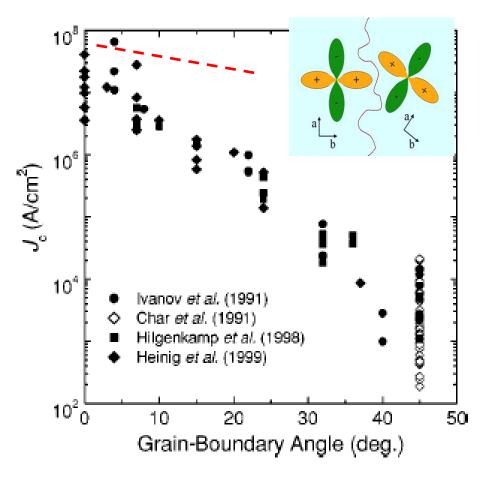
The grain boundary problem in cuprates

16^o [001] tilt grain boundary in YBCO



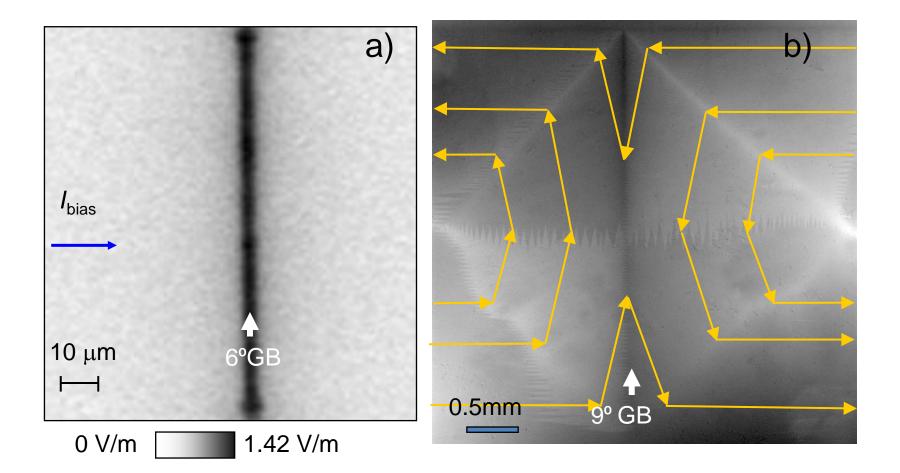


 $J_{c}(\theta) = J_{0}\cos^{2}2\theta$ - pure d-wave scenario is too weak to explain the observed exponential decrease of $J_{c}(\theta)$



X. Song et al. Nature Mat. 4, 470 (2005)

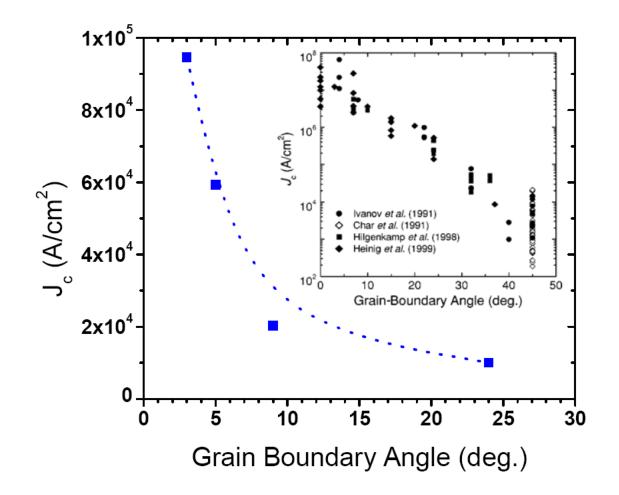
Current blocking revealed by scanning laser micrscopy and magneto-optical imaging in Ba(Fe_{1-x}Co_x)₂As bicrystals (x=0.16)



D. Abraimov, 2009

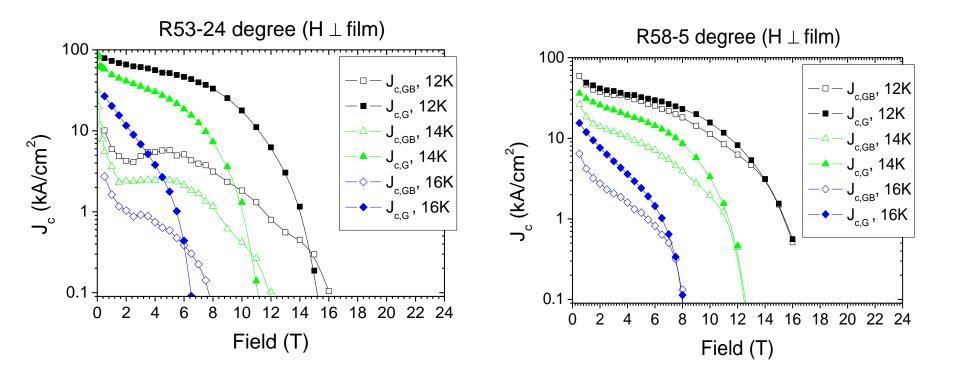
A. Polyanskii, 2009

Rapid drop of J_c with the misorientation angle measured by transport (S. Lee et al, arXiv: 0907.3741)



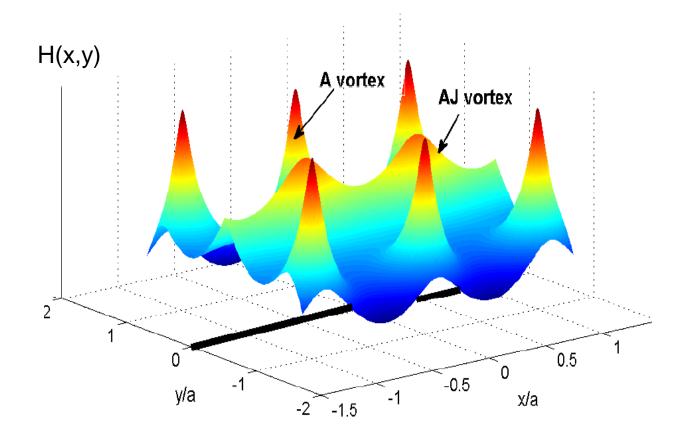
Similar ratio of $J_c (24^\circ)/J_d \sim 2 \times 10^{-4}$ indicates similar suppression of the OP on grain boundaries in YBCO and 122 pnictides

Critical currents of GBs in magnetic field



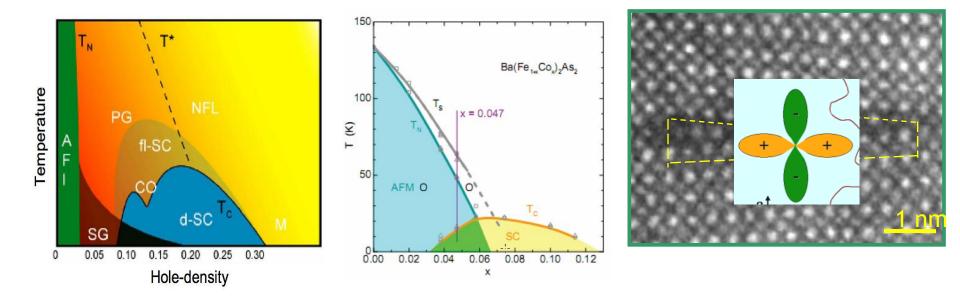
Very similar to the behavior observed on YBCO grain boundaries

Vortices on grain boundaries



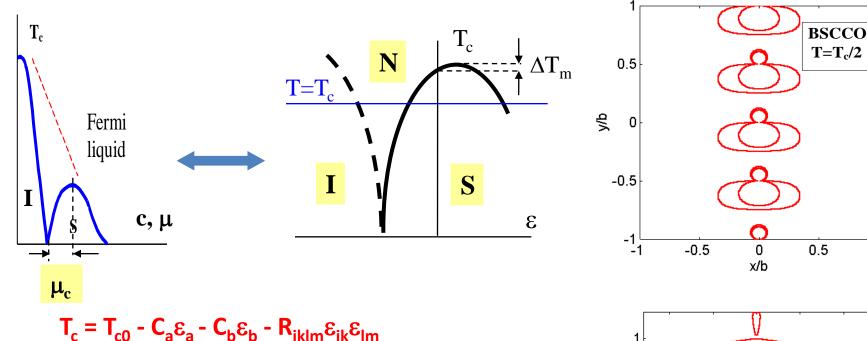
Pinning of vortices on GB by vortices in the grains

Similarities of cuprates and pnictides

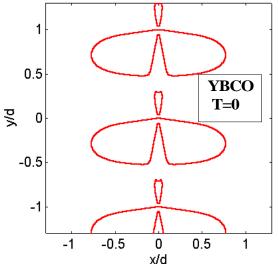


- short coherence length, $\xi \approx$ 1-2 nm
- charging and strains effects of dislocation cores
- competing orders: nonsuperconducting AF phase precipitates on GB
- low carrier density \Rightarrow long Thomas Fermi screening length $I_{TF} \approx 1-2$ nm

Strain effects at grain boundaries



- Strain-induced dielectric and normal regions near dislocation cores.
- Anisotropic T_c(ε) for YBCO (C_a ≈ C_b ~ 300K). Isotropic T_c(ε) for BSCCO (C_a ≈ C_b ~ 300K)



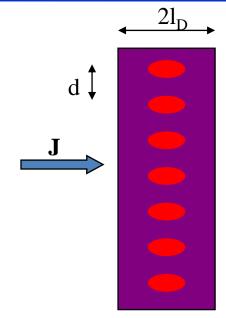
AG and E. Pashitskii, PRB, 56, 6213 (1987).

Current Channels and Charging Effects

- Charged coupling of dielectric/metallic core regions of size ~ b
- Superconductivity suppression in the space charge layer of thickness 2l_D ~ ξ₀

AG and E. Pashitskii, PRB 57, 13875 (1998); H. Hilgenkamp and J. Mannhart, APL 73, 265 (1998); RMP 74, 485 (2002)

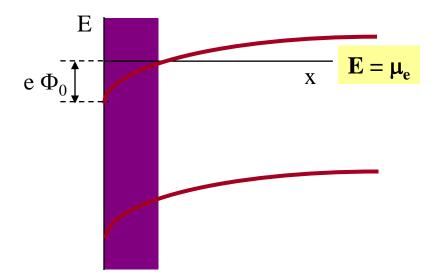
<u>"Transistor" model of GB: μ + eΦ = const</u>



 $d/2\pi$

$$\Phi_0 \cong -\frac{ZN_0\zeta b(1-2\sigma)^2 l_D \ln(d/r_i)}{4(1-\sigma)^2 \kappa_{\infty}} \sin\frac{\theta}{2}$$

 Zone bending near GB: shift toward the nonsuperconducting AF state.



Peculiarities and open questions of superconductivity in oxypnictides

- Mechanism of superconductivity the nature of the pairing glue
- Why strong magnetism does not kill s-wave superconductivity and why nonmagnetic impurities do not suppress T_c?
- How far can H_{c2}(T) go and what is the behavior of H_{c2}(T) at low temperatures? Any new states due to paramagnetic effects (FFLO state?).
- Vortex physics in pnictides. Pinning, critical currents and irreversibility fields. Effect
 of magnetism on vortex behavior.
- Proximity of SC state to AF semimetal, short coherence length, long screening length: weak linked grain boundaries block current