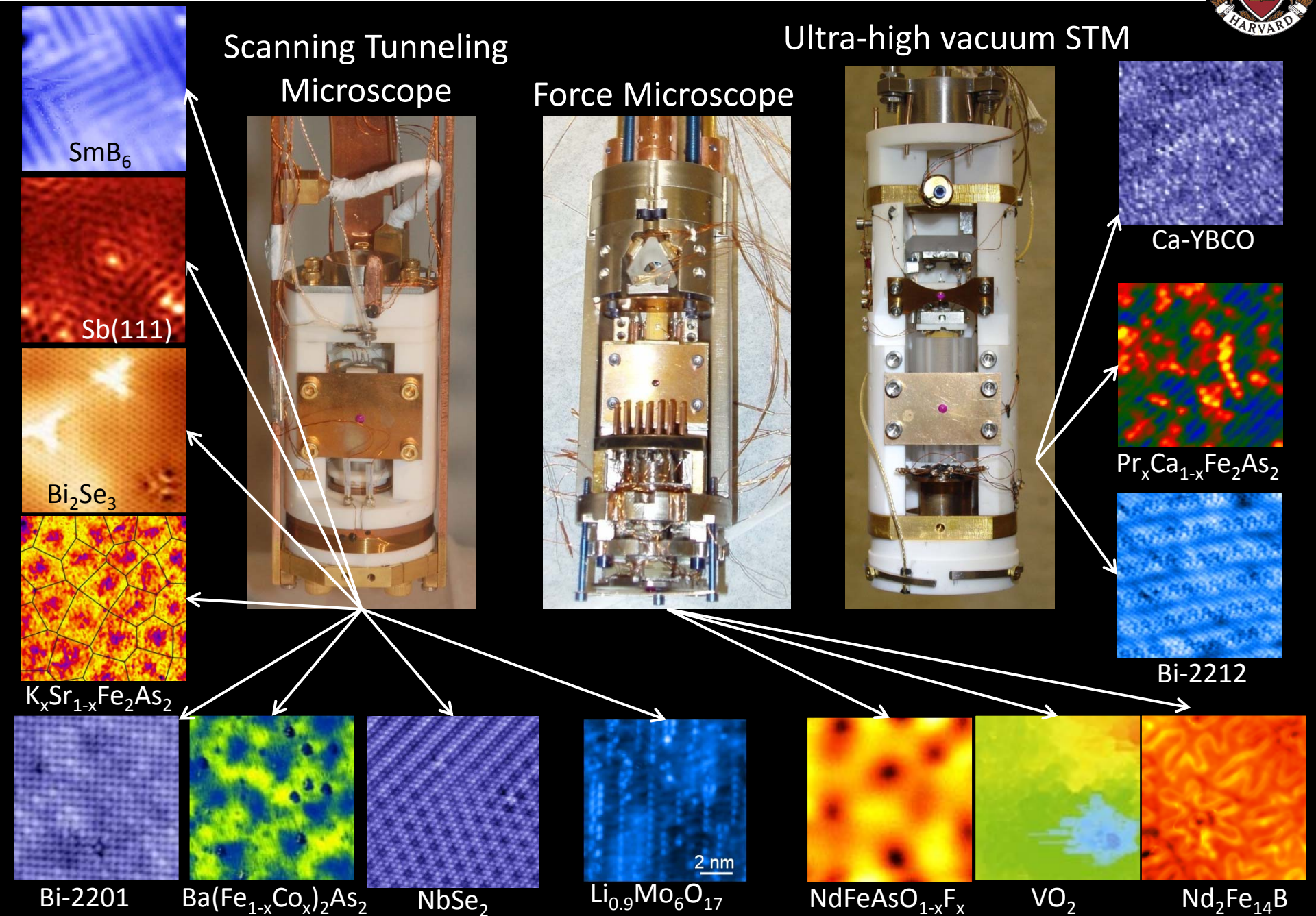
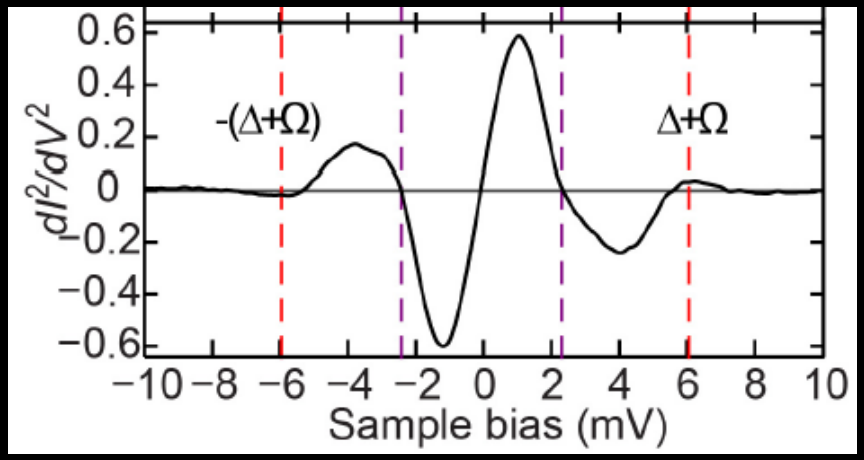
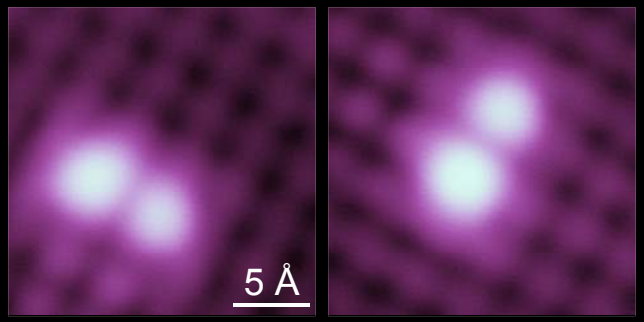
Hoffman Lab Local Probes

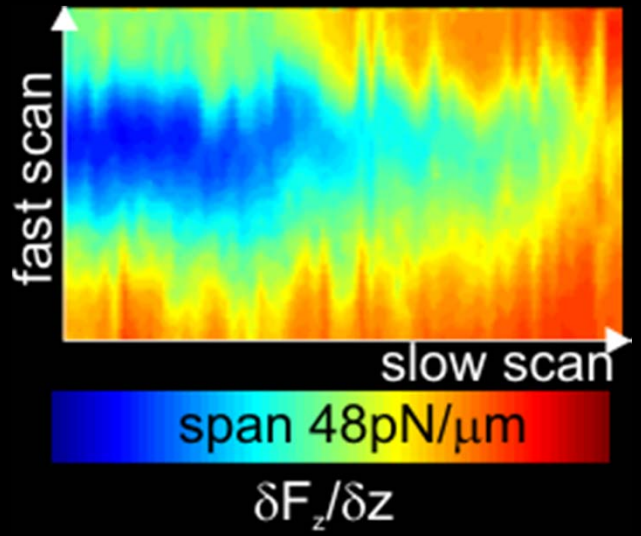


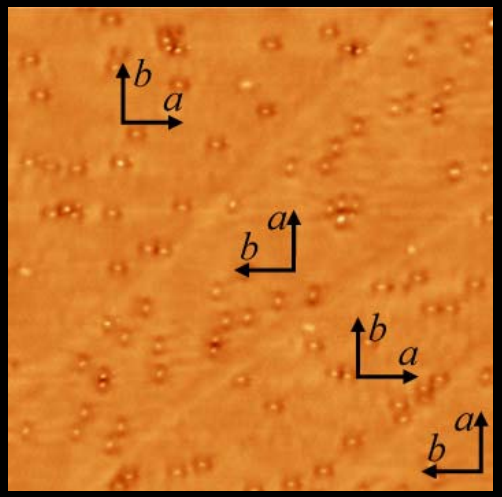
Inhomogeneity in Fe-based superconductors: Bosons, twin boundaries, defects, dopants, and vortices

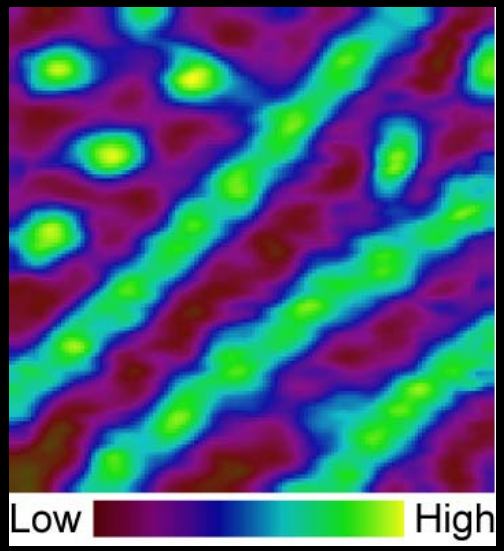
Jenny Hoffman











Contributors

FeSe

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PRL 109, 137004 (2012)
arxiv:1308.2155

$K_xSr_{1-x}Fe_2As_2$

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Nan-Lin Wang

PRB 87, 214519 (2013)

$Pr_xCa_{1-x}Fe_2As_2$

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Dennis Huang
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Bing Lv
Ching-Wu (Paul) Chu

PRB 87, 201108 (2013)

$NdFeAsO_{1-x}F_x$

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Magdalena Huefner
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Stella Kim
Ruslan Prozorov
Paul Canfield

(in preparation)

Review articles:

1. *"Spectroscopic scanning tunneling microscopy insights into Fe-based superconductors"*
   Hoffman, Reports on Progress in Physics 74, 124513 (2011)
2. *"Pairing insights in iron-based superconductors from scanning tunneling microscopy"*
   Song + Hoffman, Current Opinion in Solid State and Materials Science 17, 39 (2013)
3. *"Interplay of chemical disorder and electronic inhomogeneity in unconventional superconductors"*
   Zeljkovic + Hoffman, Physical Chemistry Chemical Physics 15, 13462 (2013)

Thanks to: BSF, NSEC, Harvard, NSF, Alfred P. Sloan Foundation

Outline

Boson mode

- seen in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$, LiFeAs, $NaFe_{1-x}Co_xAs$, and now FeSe
- $\Omega(r)$ correlates with $\Delta(r)$ in FeSe (*c.f.* anti-correlation in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$)

$$\Delta(r) = \Omega(r)\exp\left(\frac{-\Omega(r)}{2N_0 g^2}\right)$$

Twin boundaries

- repel vortices in $Ba(Fe_{1-x}Co_x)_2As_2$, but pin vortices in FeSe
- enhance pnictogen/chalcogen height?

Fe site defects

- geometric dimers
- electronic dimers cause transport anisotropy

Vortices

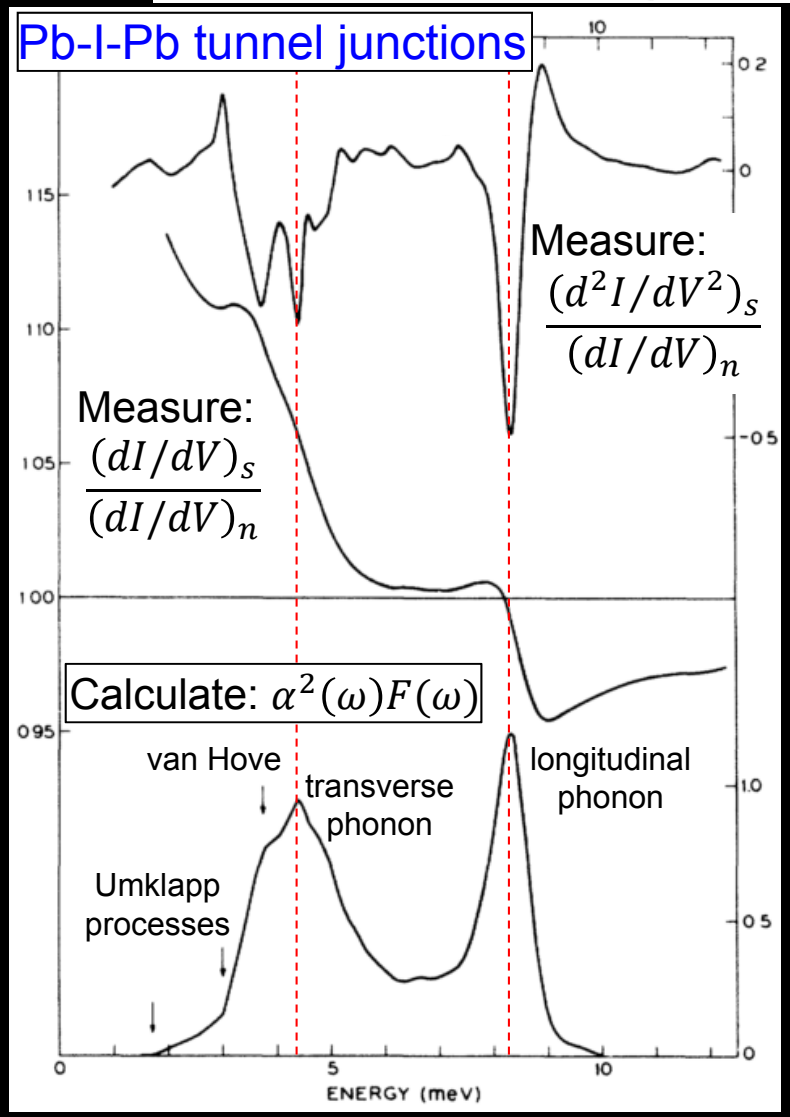
- no anisotropy observed in $NdFeAsO_{1-x}F_x$
- single-vortex pinning force ~8 picoNewtons in $NdFeAsO_{1-x}F_x$
- $\lambda \sim 500$ nm in $NdFeAsO_{1-x}F_x$

1965: Phonon coupling in Pb

VOLUME 14, NUMBER 4 PHYSICAL REVIEW LETTERS 25 JANUARY 1965

LEAD PHONON SPECTRUM CALCULATED FROM SUPERCONDUCTING DENSITY OF STATES

W. L. McMillan and J. M. Rowell
Bell Telephone Laboratories, Murray Hill, New Jersey



$F(\omega)$ = phonon density of states

$\alpha^2(\omega)$ = coupling

How to compute $\alpha^2(\omega)F(\omega)$

1. Measure $N_s(\omega)$
2. Guess a functional form for $\alpha^2(\omega)F(\omega)$ (recalling that they are both integrals over a full BZ)

$$F(\omega) = \sum_\lambda \int \frac{d^3q}{(2\pi)^3} \delta(\omega - \omega_{q\lambda})$$

$$\alpha^2(\omega)F(\omega) = \int_S d^2p \int_{S'} \frac{d^3p}{2\pi^2 v_{\mathrm{F}}'} \sum_\lambda g_{pp'\lambda} \times \delta(\omega - \omega_{p-p'\lambda}) \Big/ \int_S d^2p,$$

where $g_{pp'\lambda}'$ is the dressed electron-phonon coupling constant, $\omega_{q\lambda}$ is the phonon energy for polarization λ and wave number q (reduced to the first zone), and v_{F} is the Fermi velocity. The two surface integrations are performed over the Fermi surface.

3. Plug in the guessed $\alpha^2(\omega)F(\omega)$ to compute $\Delta(\omega)$

$$\varphi(\omega) = \int_{\Delta_0}^{\omega_c} d\omega' \, \mathrm{Re}\left[\frac{\Delta'}{(\omega'^2 - \Delta'^2)^{1/2}}\right] \times \left\{ \int d\omega_q \, \alpha^2(\omega_q) F(\omega_q) [D_q(\omega' + \omega) + D_q(\omega' - \omega)] - U_c \right\},$$

where $D_q(\omega) = (\omega + \omega_q - i0^+)^{-1}$, $\Delta(\omega) = \varphi(\omega)/Z(\omega)$

4. Plug in the computed $\Delta(\omega)$ to compute $N_s(\omega)$ and compare back to measured $N_s(\omega)$

$$\frac{N_s(\omega)}{N(0)} = \mathrm{Re}\left\{ \frac{|\omega|}{[\omega^2 - \Delta^2(\omega)]^{1/2}} \right\}$$

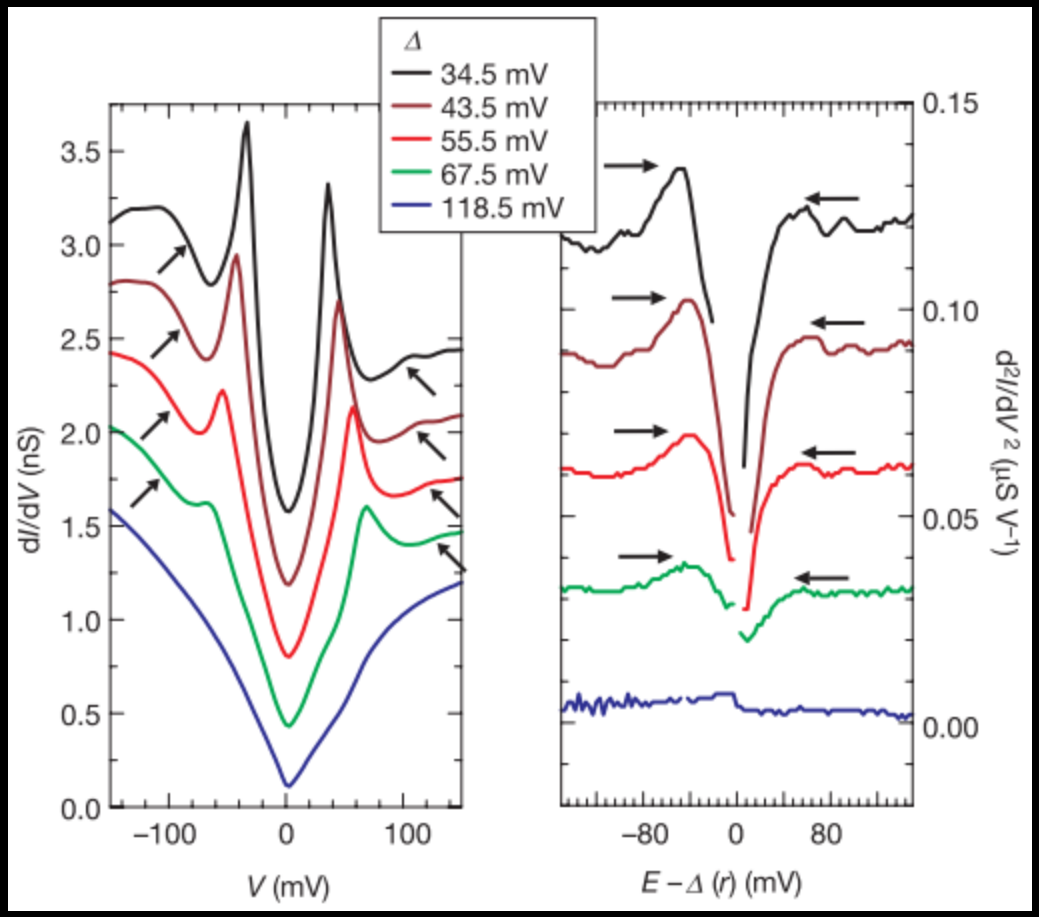
5. Compute the error and iterate

$$\delta[\alpha^2(\omega)] = \int d\omega' \left\{ \frac{\delta N(\omega')}{\delta[\alpha^2(\omega)F(\omega)]} \right\}^{-1} \times [N_s^{\mathrm{expt}}(\omega') - N_s^{\mathrm{calc}}(\omega')]$$

McMillan & Rowell, PRL 14, 108 (1965)

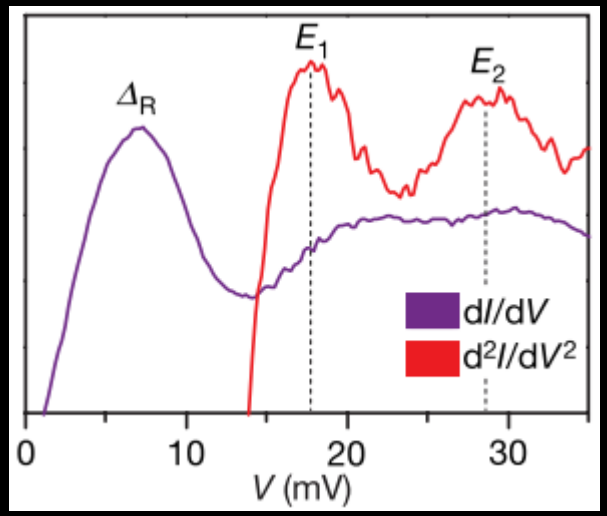
Electron-boson coupling in cuprates

$Bi_2Sr_2CaCu_2O_{8+d}$ (T_c^{max} = 91K)



Lee, Nature 442, 546 (2006)

$Pr_{0.88}LaCe_{0.12}CuO_4$ (T_c=24K)

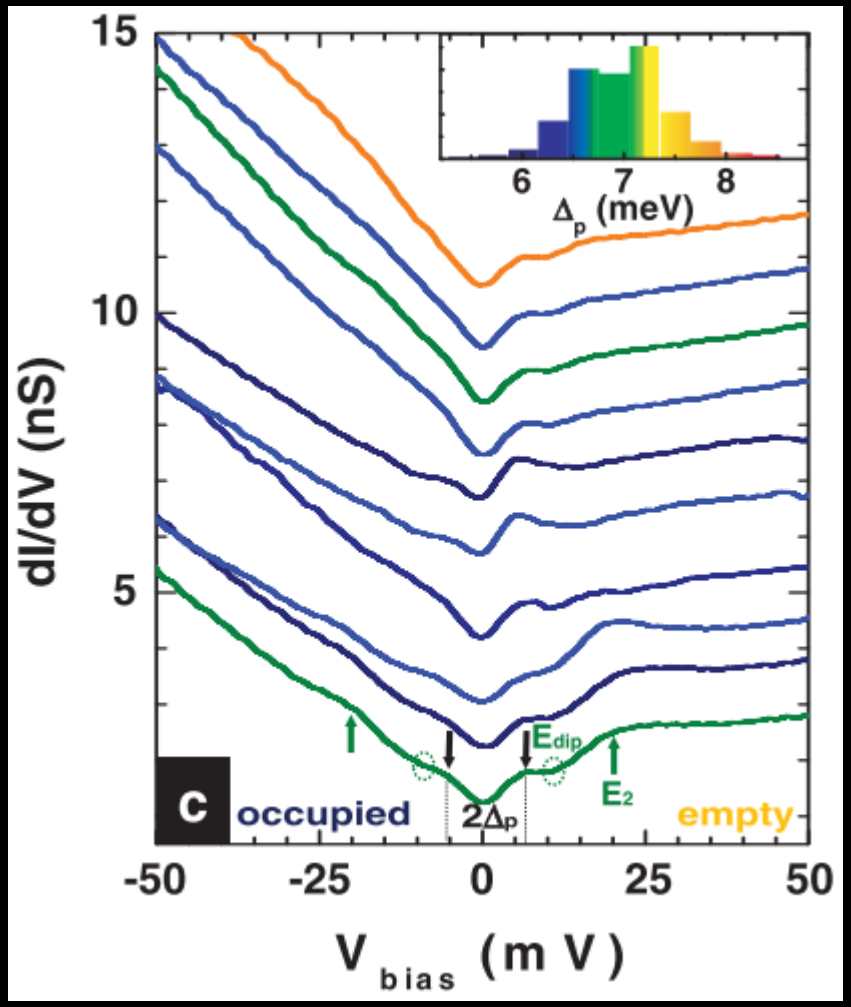


Niestemski, Nature 450, 1058 (2007)

$$\Omega = E \text{ (peak in } d^2I/dV^2) - \Delta$$

1111 Fe-superconductors

$SmFeAsO_{0.8}F_{0.2}$ (T_c=45K)

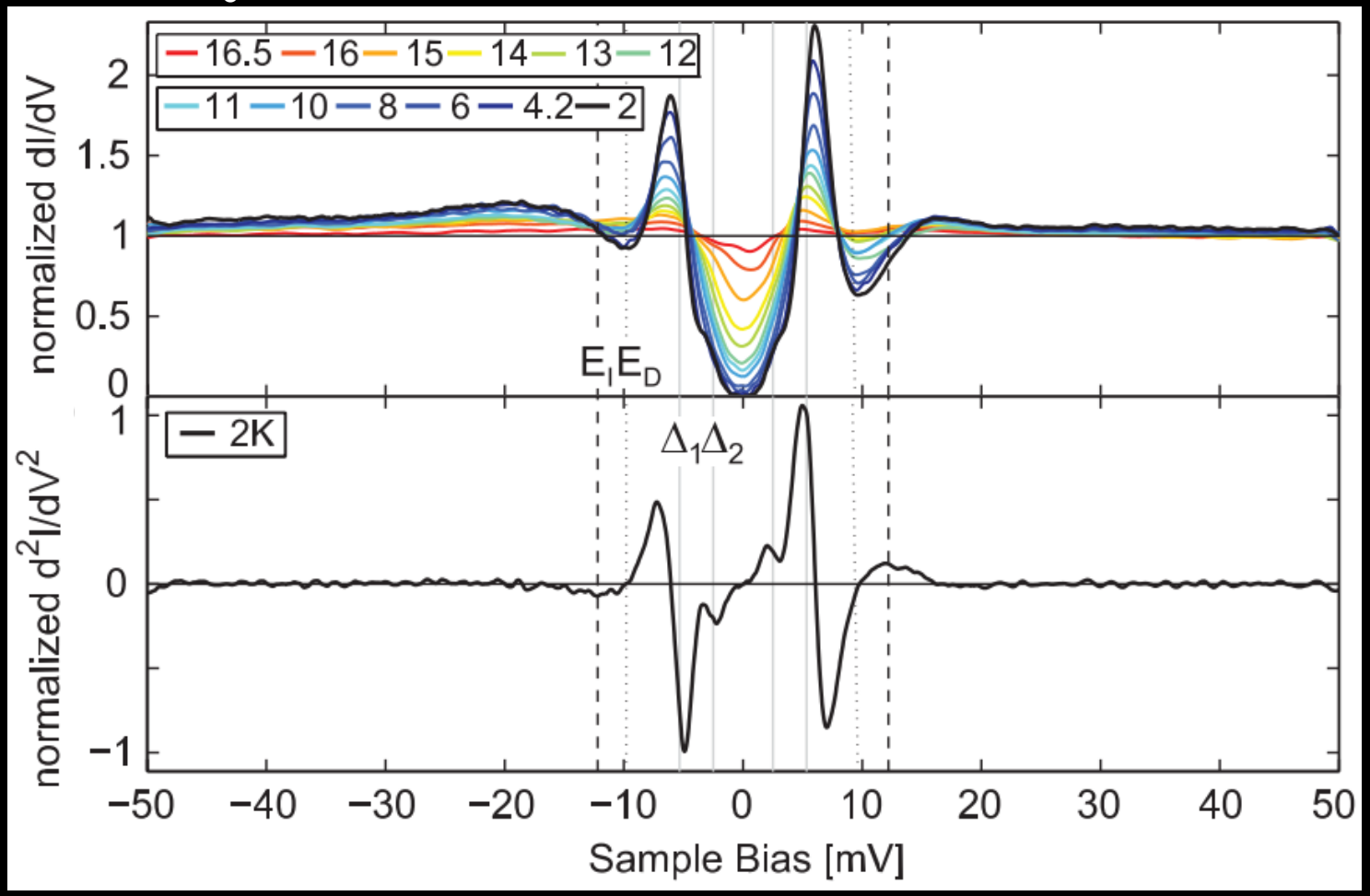


Fasano, PRL 105, 167005 (2010)

$$\Omega = E\ (\text{dip in } dI/dV) - \Delta$$

111 Fe-superconductors

LiFeAs (T_c=17K)



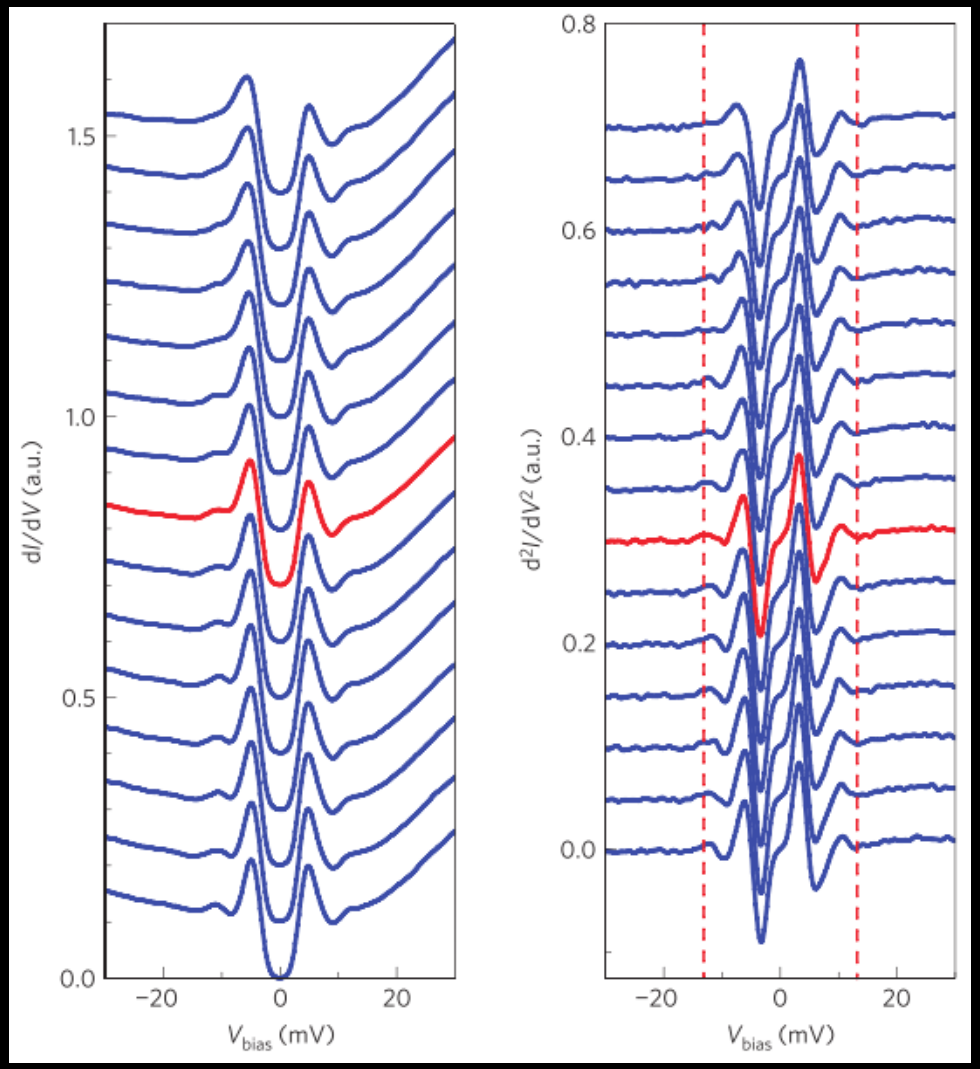
Chi, PRL 109, 087002 (2011)

$$\Omega = E\ (\text{dip in } dI/dV) - \Delta$$

111 Fe-superconductors

$Na(Fe_{0.975}Co_{0.025})As$ (T_c=21 K)

E (hump in dI/dV)
= 13.3 ± 0.8



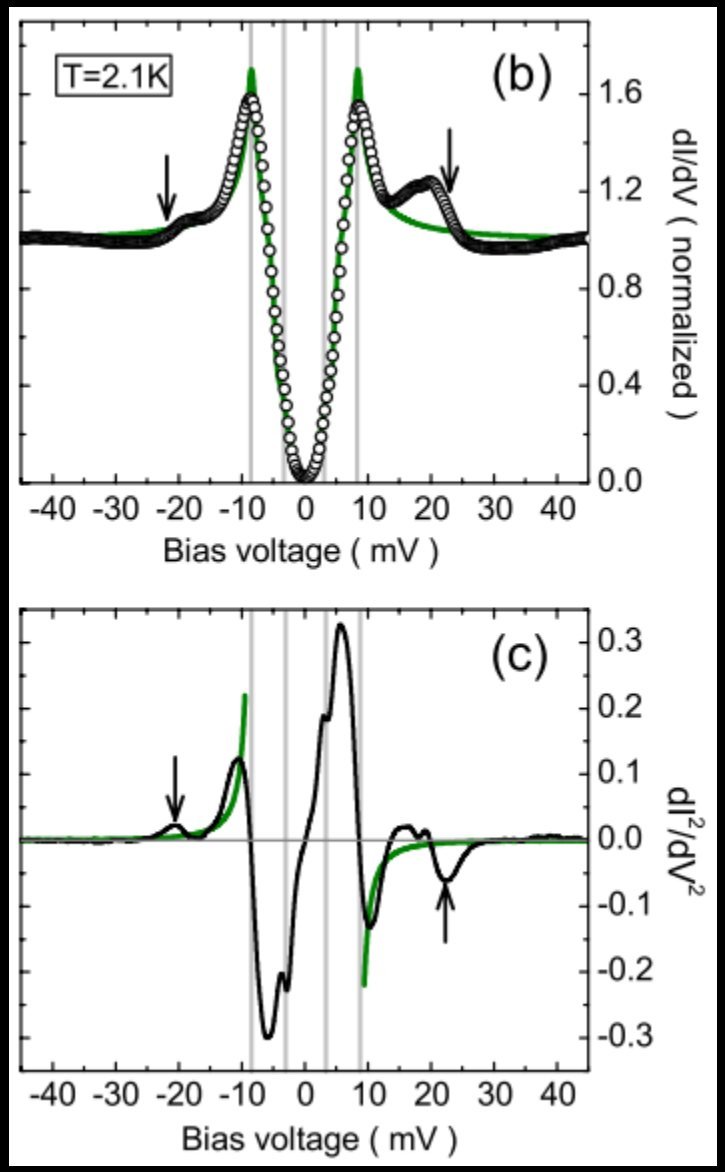
E (dip in d^2I/dV^2)
= 13.3 ± 0.8 (main text)
= 13.5 (figure caption)

Shan, Nat Phys 9, 42 (2012)

$\boxed{\Omega = E \text{ (dip in } d^2I/dV^2) - \Delta}$ **???**

122 Fe-superconductors

$Ba_{0.6}K_{0.4}Fe_2As_2$ (T_c=38K)



$$\Omega = E \text{ (dip in } d^2I/dV^2) - \Delta$$

Shan, PRL 108, 227002 (2012)

Forward modeling

Solve the self-consistent Eliashberg equations for $Ba_{0.6}K_{0.4}Fe_2As_2$:

$$G_a^{-1}(\varepsilon, i\omega_n) = i\omega_n \tau_0 - \varepsilon\tau_3 - \Sigma_a(i\omega_n)$$

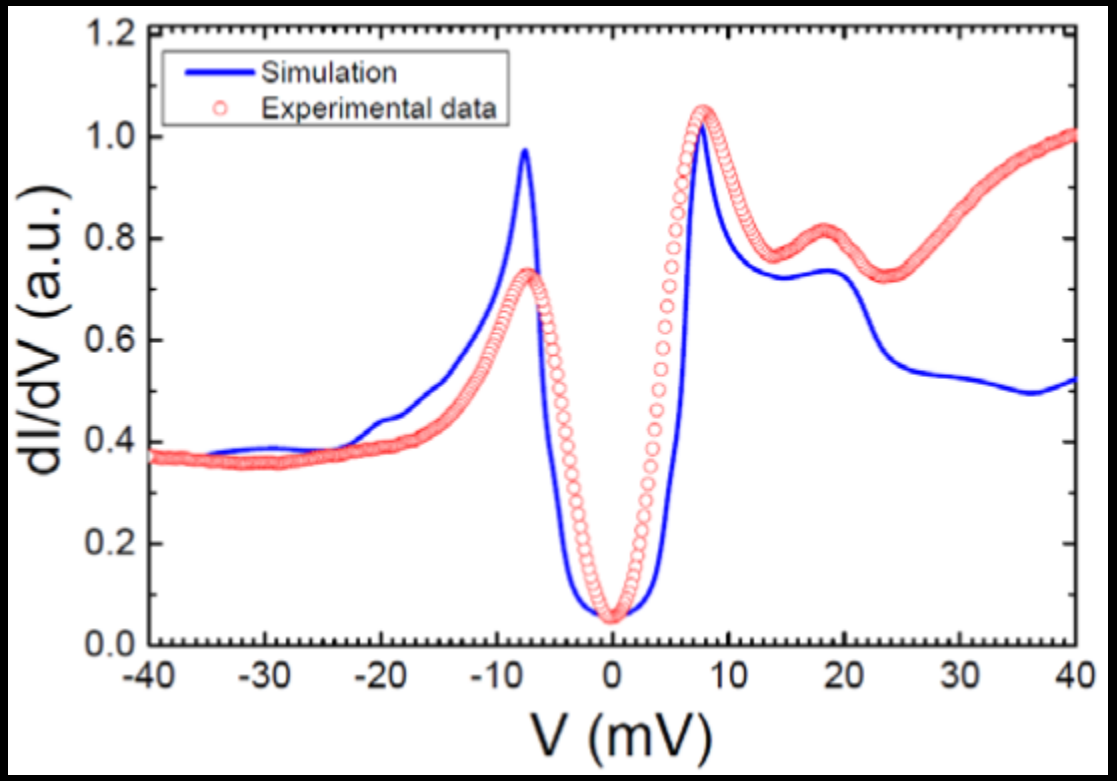
$$\Sigma_a(i\omega_n) = \sum_b g_{ab}^2 \int d\varepsilon \rho_b(\varepsilon) T \sum_{\omega_m} G_b(\varepsilon, i\omega_m) \int_0^\infty d\nu B(\nu) \frac{2\nu}{\nu^2 + (\omega_n - \omega_m)^2}$$

coupling constants: pick 2 values for coupling of the 2 h & 2 e bands that seem to work

simplified DOS: constant A_h for h bands, $A_e\sqrt{\varepsilon - \varepsilon_{\min}}$ for e bands

Lorentzian spin mode at 14.5 meV

Free parameters: couplings $\lambda_{e_1h_1}$, $\lambda_{e_2h_2}$, $B(\nu)$ center & width, A_h, A_e, $\varepsilon_{\min}$, elastic scattering γ



Conclusion:

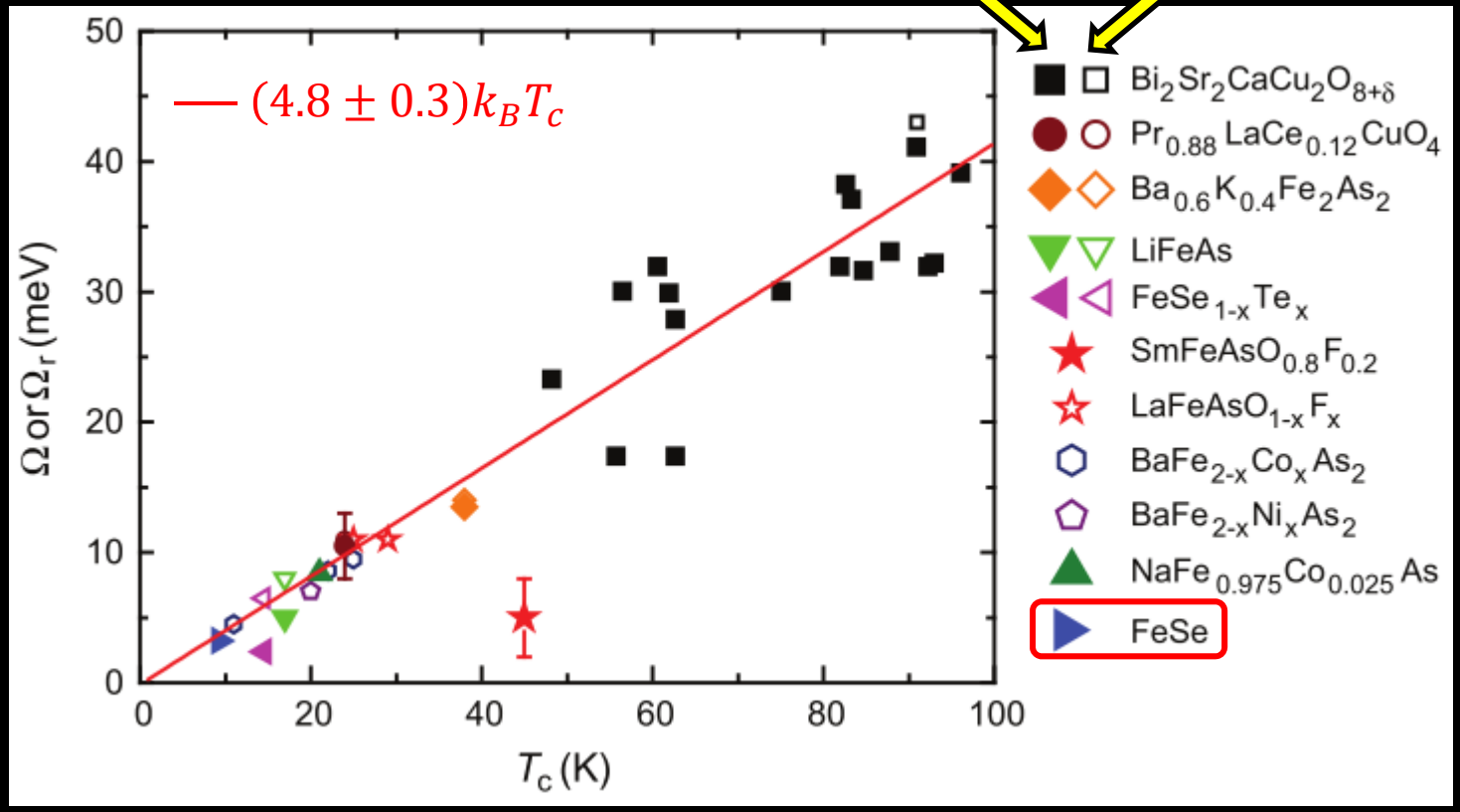
They have a plausible but very simple model which qualitatively reproduces the data, analogous to Schrieffer, Scalapino & Wilkins, PRL 10, 336 (1963),
but they didn't go backwards to actually compute the coupling $\sqrt{\rho_\alpha(0)\rho_\beta(0)g_{\alpha\beta}^2 B(\nu)}$
which is the analog of $\alpha^2(\omega)F(\omega)$
as in McMillan & Rowell, PRL 14, 108 (1965).

Shan, Nat Phys 9, 42 (2012)

Ω in cuprates and Fe-superconductors

solid symbols = Ω
(from STM)

open symbols = Ω_r
(from neutron scattering)



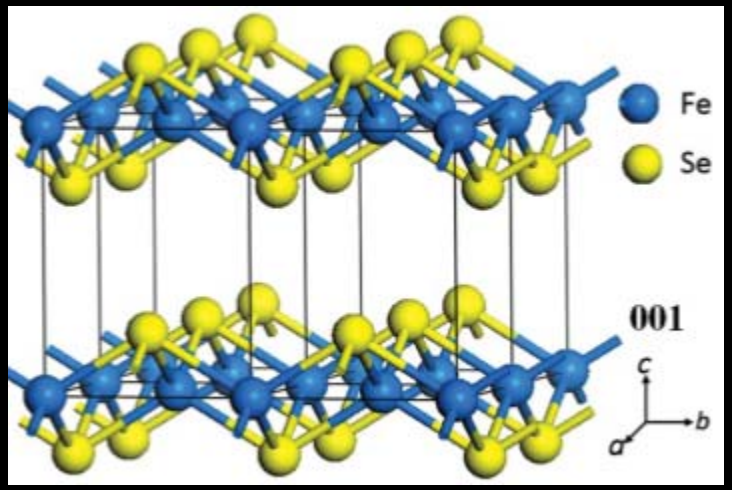
E (dip in dI/dV)
E (peak in d^2I/dV^2)
E (dip in d^2I/dV^2)
E (dip in dI/dV)
E (peak in d^2I/dV^2)
E (dip in dI/dV)

E (dip in d^2I/dV^2)
E (peak in d^2I/dV^2)

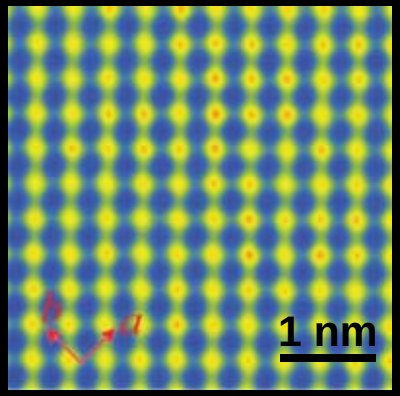
Song + Hoffman, Current Opinion in Solid State and Materials Science 17, 39 (2013)

Boson in 11 superconductor: FeSe

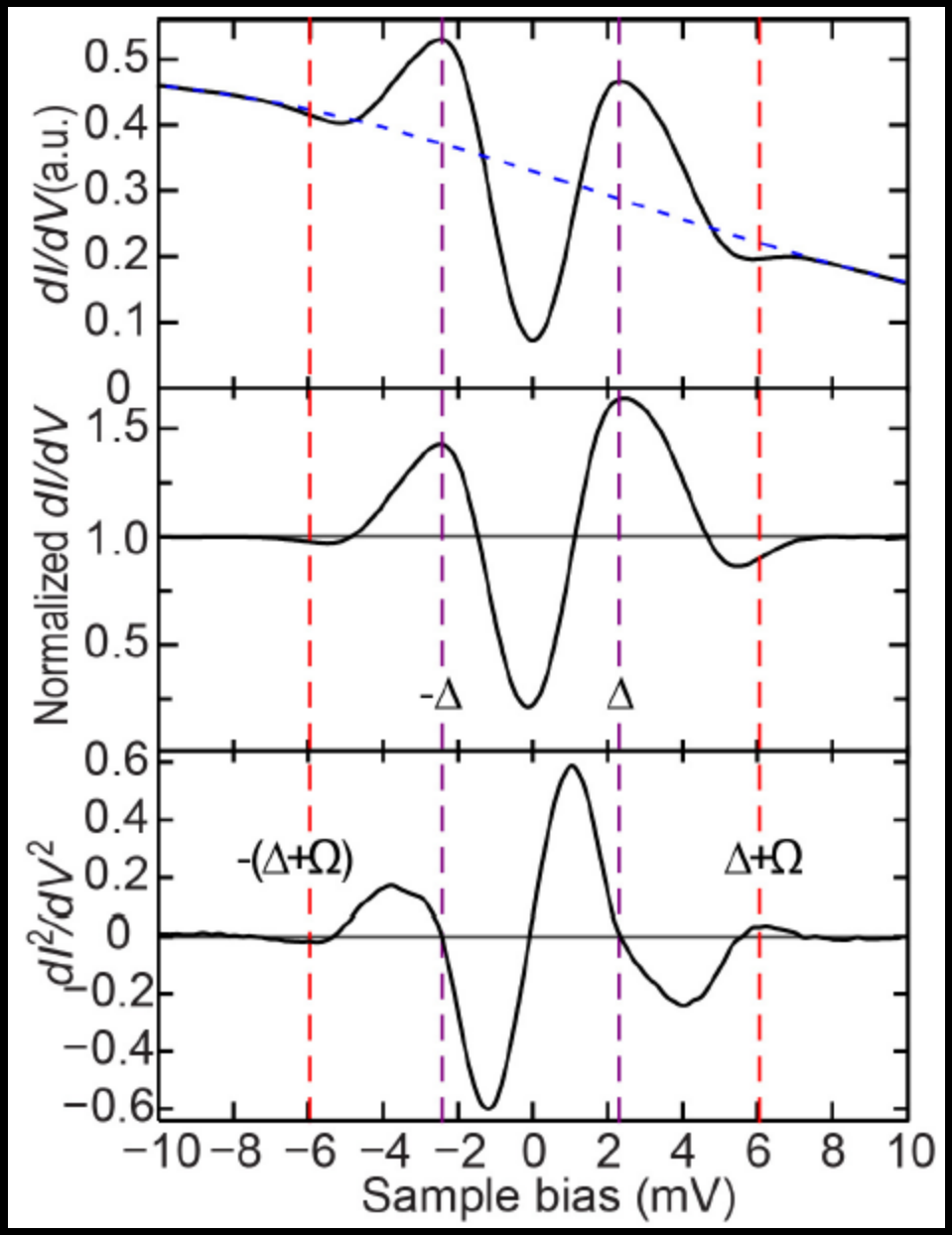
FeSe film on graphene (T_c~8K)



STM topography

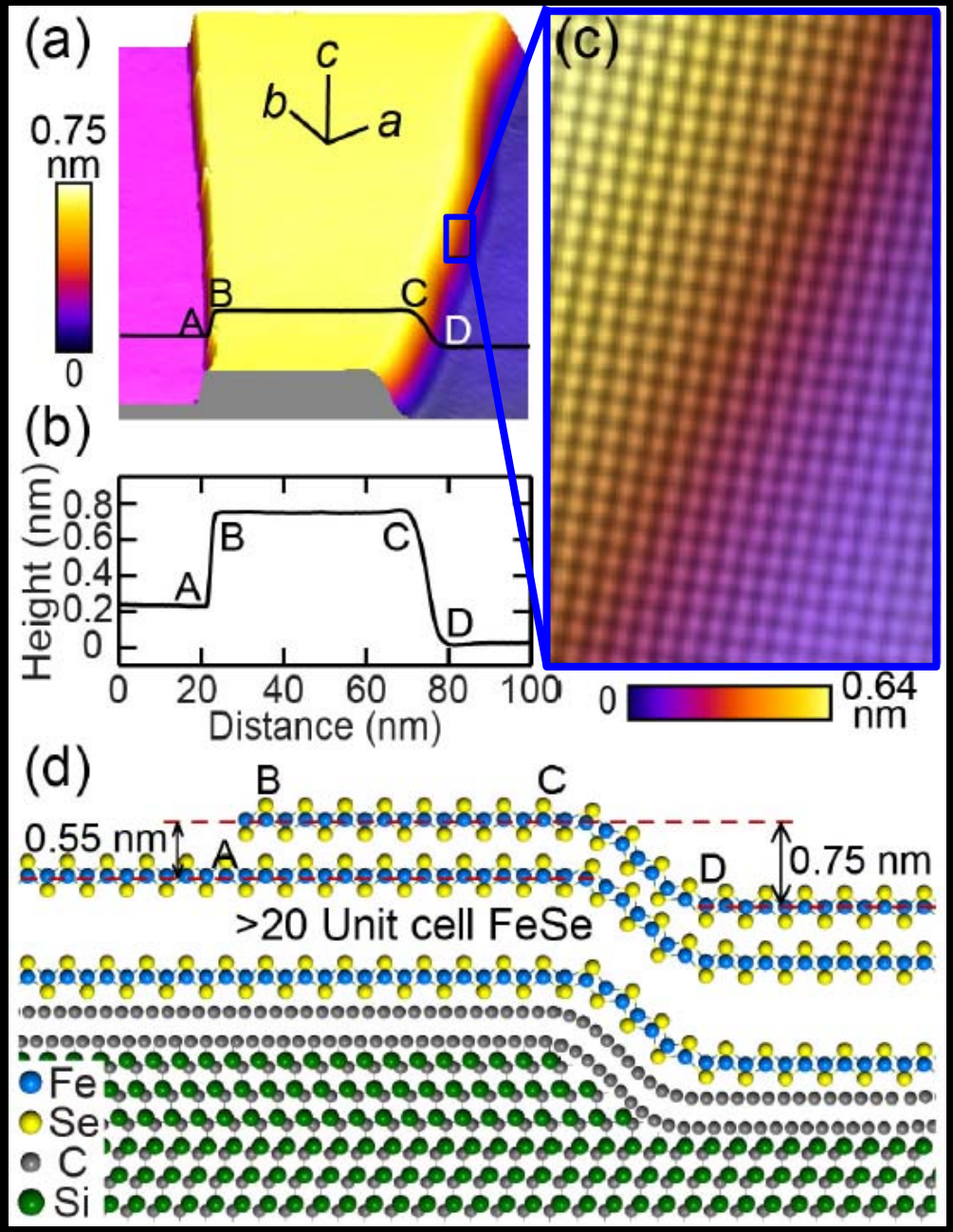


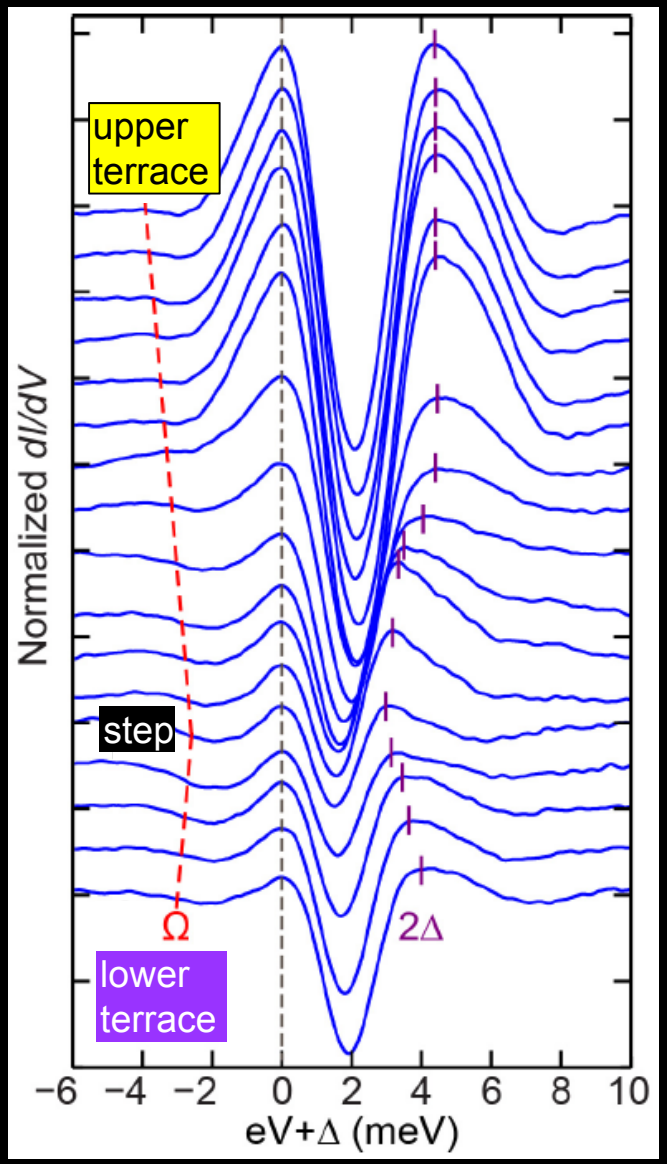
$$\Omega = E\ (\text{peak in } d^2I/dV^2) - \Delta$$



Song, arxiv:1308.2155

Tensile strain reduces Δ and Ω in FeSe

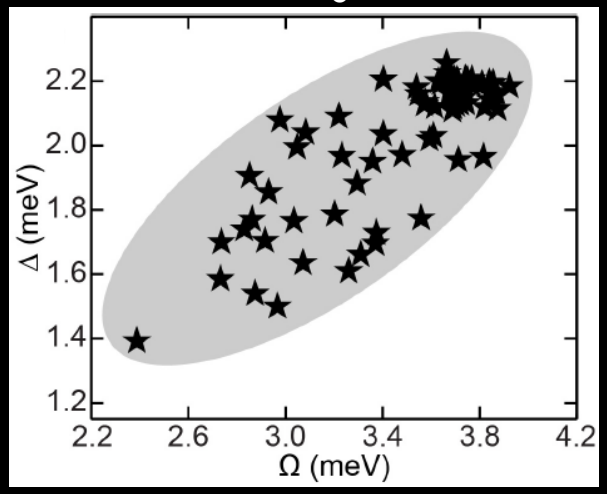




Song, arxiv:1308.2155

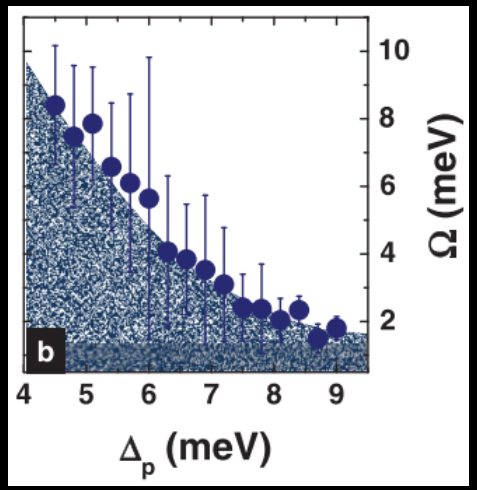
Fe-SCs: local relation between $\Delta(r)$ and $\Omega(r)$

FeSe (T_c=8K)



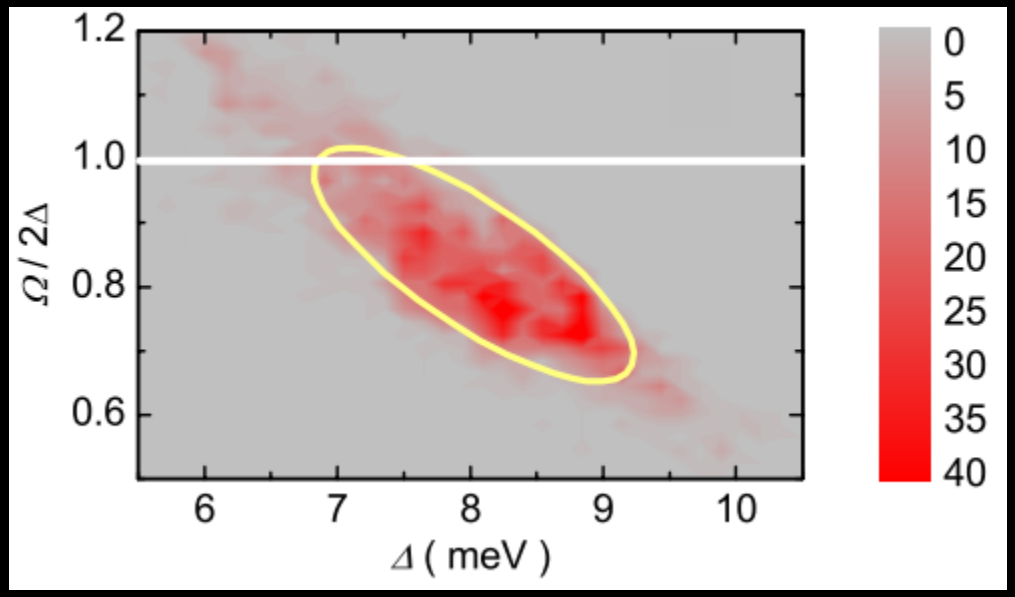
Song, arxiv:1308.2155

$SmFeAsO_{0.8}F_{0.2}$ (T_c=45K)



Fasano, PRL 105 167005 (2010)

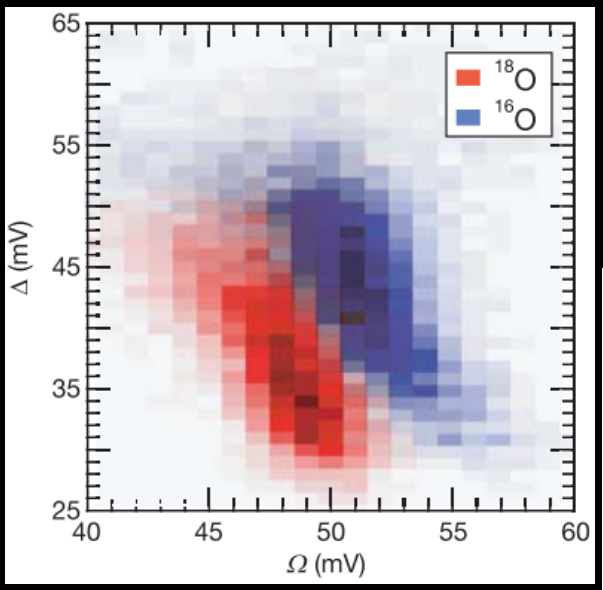
$Ba_{0.6}K_{0.4}Fe_2As_2$ (T_c=38K)



Shan, PRL 108, 227002 (2012)

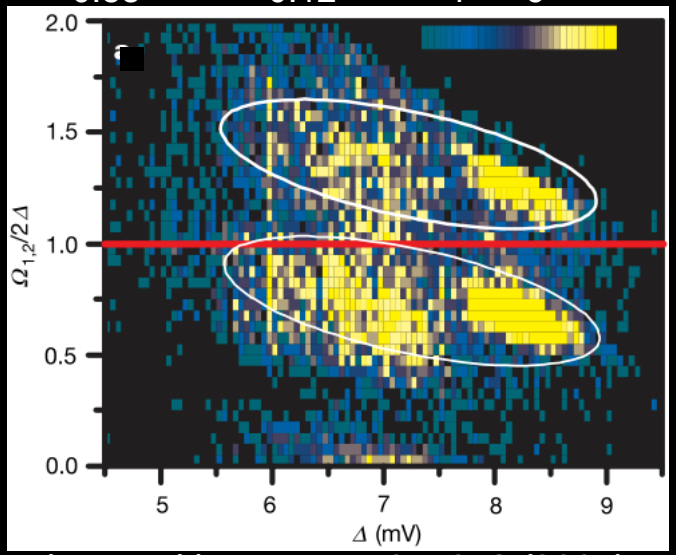
Cuprates: local relation between $\Delta(r)$ and $\Omega(r)$

Bi-2212 ($T_c^{\max} = 91\mathrm{K}$)



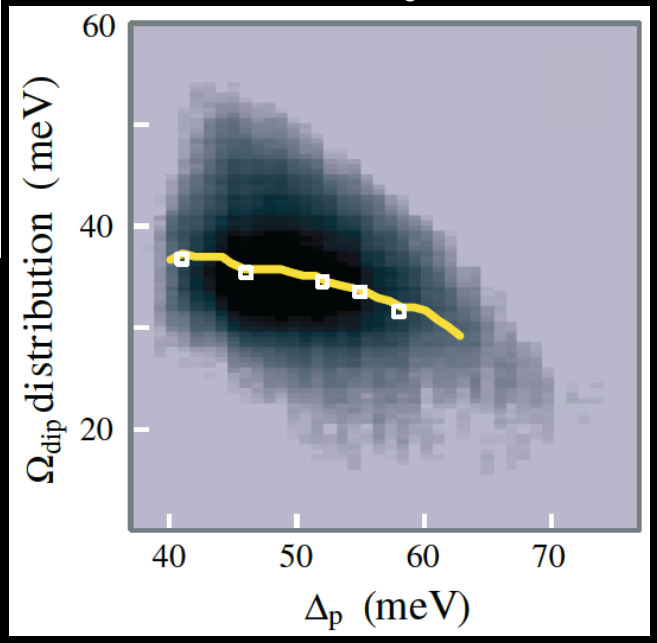
Lee, Nature 442, 546 (2006)

$Pr_{0.88}LaCe_{0.12}CuO_4$ (T_c=21K)



Niestemski, Nature 450, 1058 (2007)

Bi-2223 (T_c=110K)



Jenkins, PRL 103, 227001 (2009)

Local strong-coupling pairing

Solve the local Eliashberg equations with patch size ~2-5 nm:

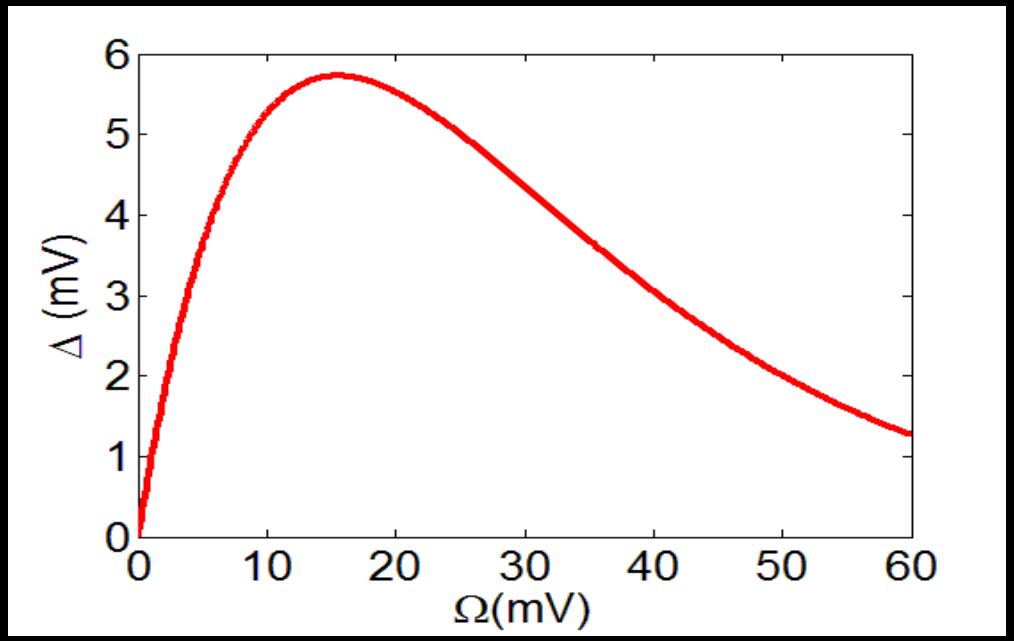
$$\Delta(r) = \Omega(r)\exp\left(\frac{-1}{N_0 g_{\mathrm{eff}}(r)}\right)$$

$g_{\mathrm{eff}}(r) =$ effective coupling constant

$$g_{\mathrm{eff}}(r) = \frac{2g(r)^2}{\Omega(r)}$$

$g(r) =$ local coupling constant

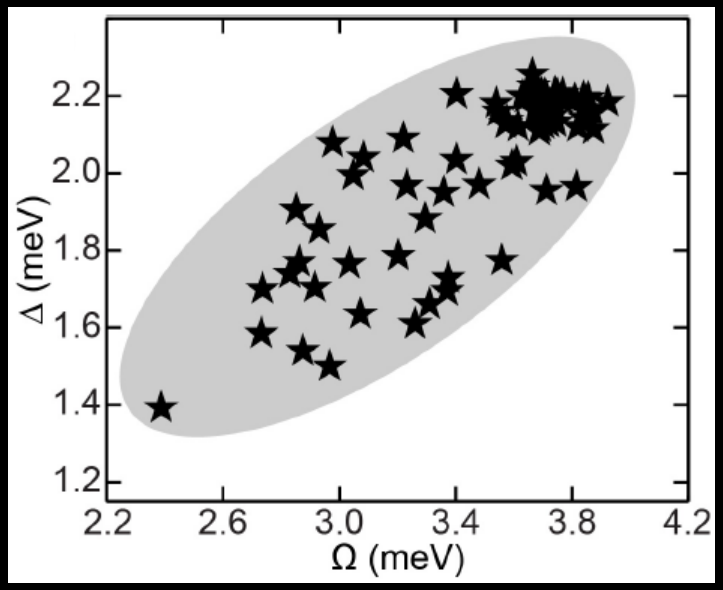
$$\boxed{\Delta(r) = \Omega(r)\exp\left(\frac{-\Omega(r)}{2N_0 g(r)^2}\right)}$$



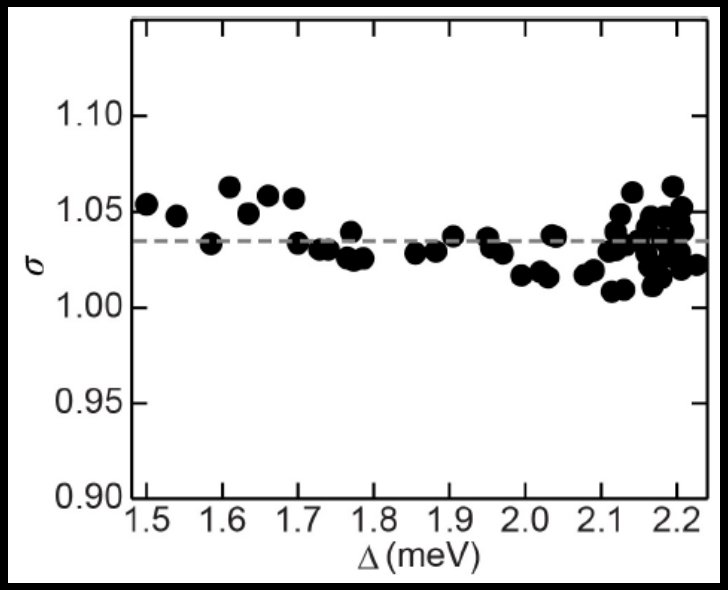
Balatsky + Zhu, PRB 74, 094517 (2006)

What about $g(r)$?

$\Omega(r)$:$\Delta(r)$ → correlation



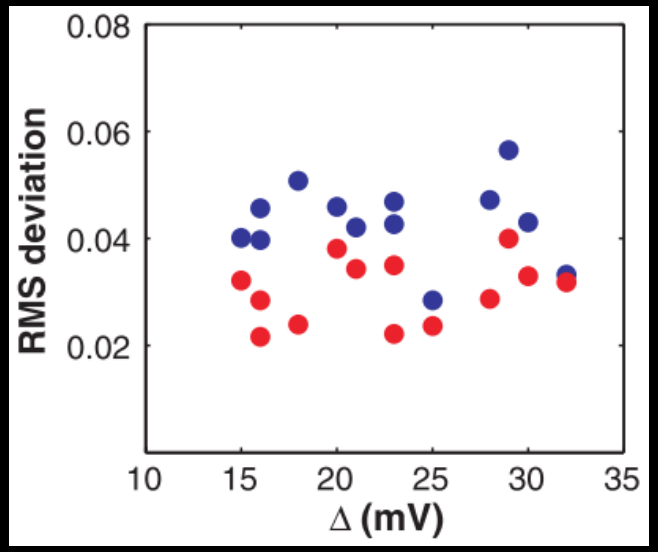
$g(r)$:$\Delta(r)$ → no correlation



Song, arxiv:1308.2155

c.f. cuprates:

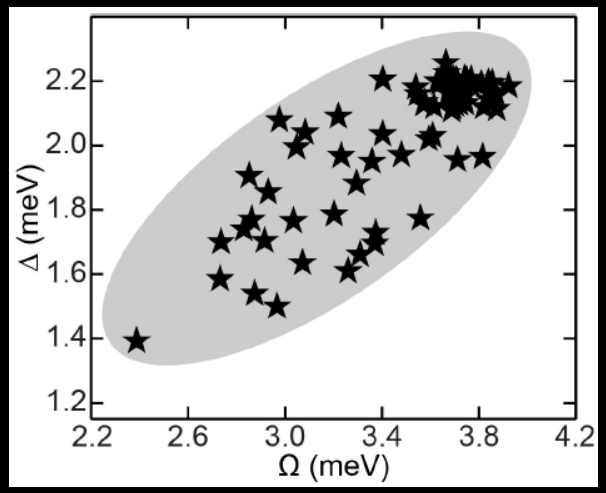
$g(r)$: $\Delta(r)$ → no correlation in $Bi_2Sr_2CaCu_2O_{8+d}$

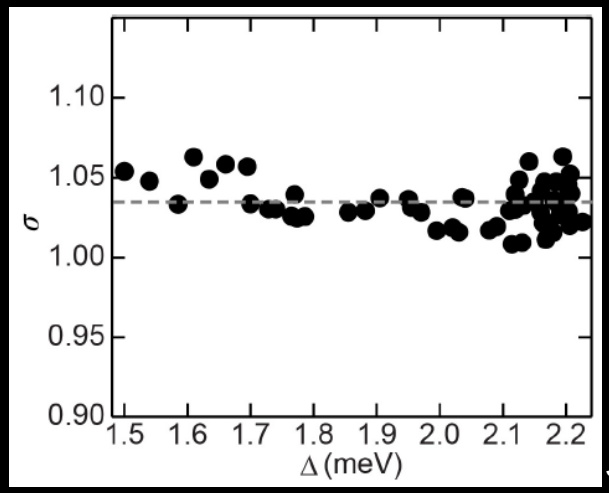


Pasupathy, Science 320, 196 (2008)

Some things I don't understand about bosons

1. Why does $\Omega(r)$ correlate with $\Delta(r)$ but $g(r)$ doesn't ?

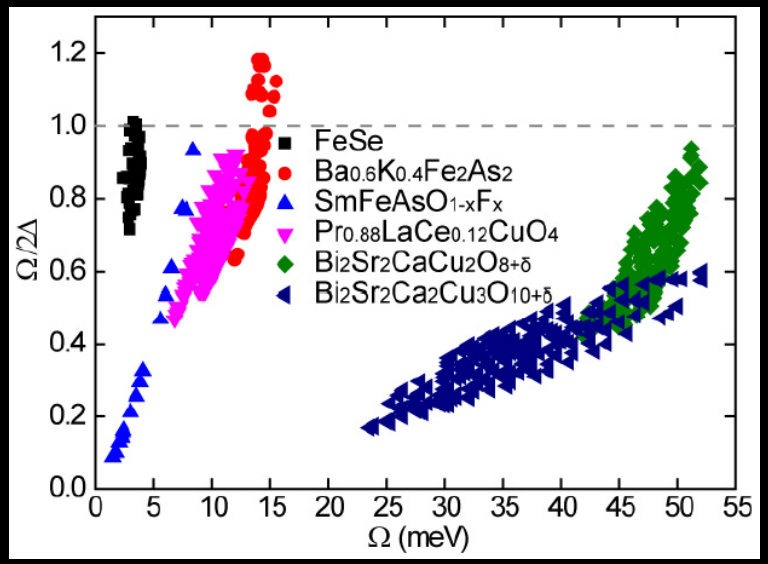




Song, arxiv:1308.2155

2. Can we invert d^2I/dV^2 to get $\Omega(\omega)$ and $g(\omega)$?

3. Use $\Delta(r) = \Omega(r)\exp\left(\frac{-\Omega(r)}{2N_0g^2}\right)$ to extract N_0g^2 in unconventional superconductors?



Outline

Boson mode

- seen in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$, LiFeAs, $NaFe_{1-x}Co_xAs$, and now FeSe
- $\Omega(r)$ correlates with $\Delta(r)$ in FeSe (*c.f.* anti-correlation in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$)

$$\Delta(r) = \Omega(r)\exp\left(\frac{-\Omega(r)}{2N_0 g^2}\right)$$

Twin boundaries

- repel vortices in $Ba(Fe_{1-x}Co_x)_2As_2$, but pin vortices in FeSe
- enhance pnictogen/chalcogen height?

Fe site defects

- geometric dimers
- electronic dimers cause transport anisotropy

Vortices

- no anisotropy observed in $NdFeAsO_{1-x}F_x$
- single-vortex pinning force ~8 picoNewtons in $NdFeAsO_{1-x}F_x$
- $\lambda \sim 500$ nm in $NdFeAsO_{1-x}F_x$

Twin boundaries in superconductors

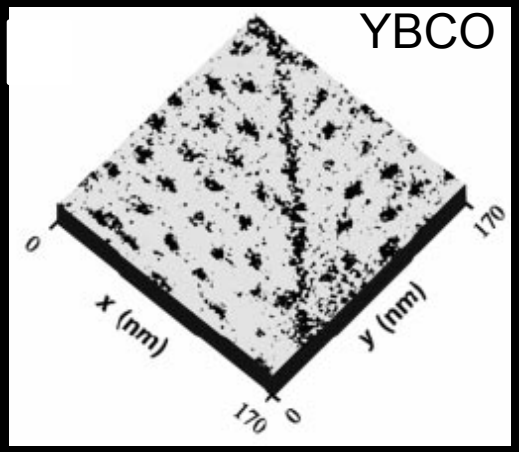
Conventional

Superconductors	T_c(TB) —T_{c0}(bulk)
Sn	0.04 K (1.1%)
In	0.01 K (0.3%)
Nb	0.11 K (1.2%)
Re	0.006 K (0.4%)
Ti	0.003 K (0.1%)

TBs enhance T_c

Khlyustikov, Adv. Phys. 36, 271 (1987)

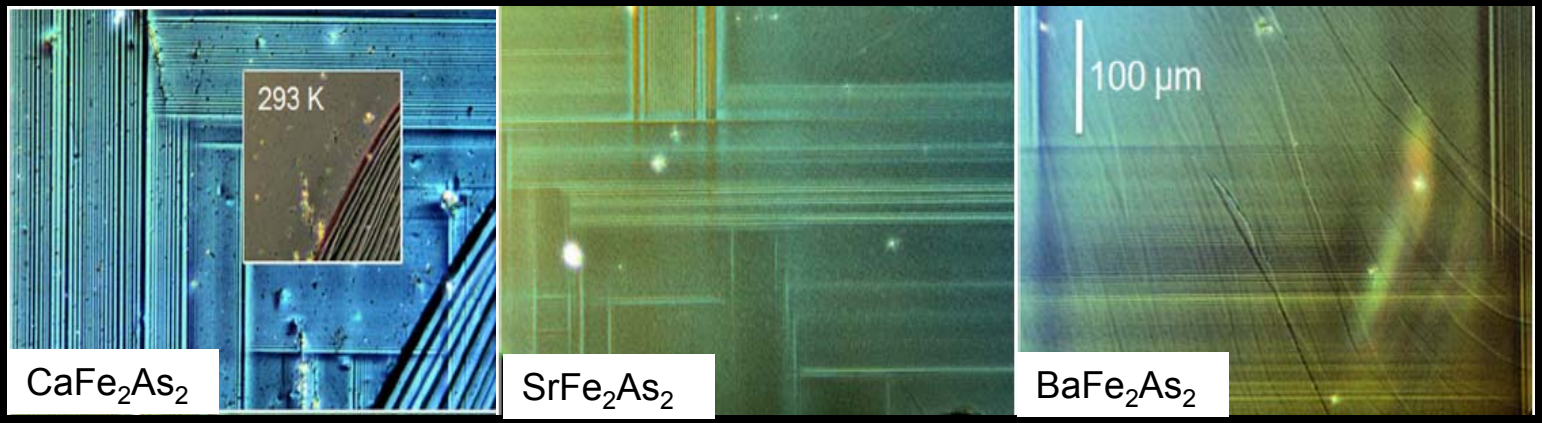
Cuprates



TBs pin vortices

Maggio-Aprile, Nature 390, 487 (1997)

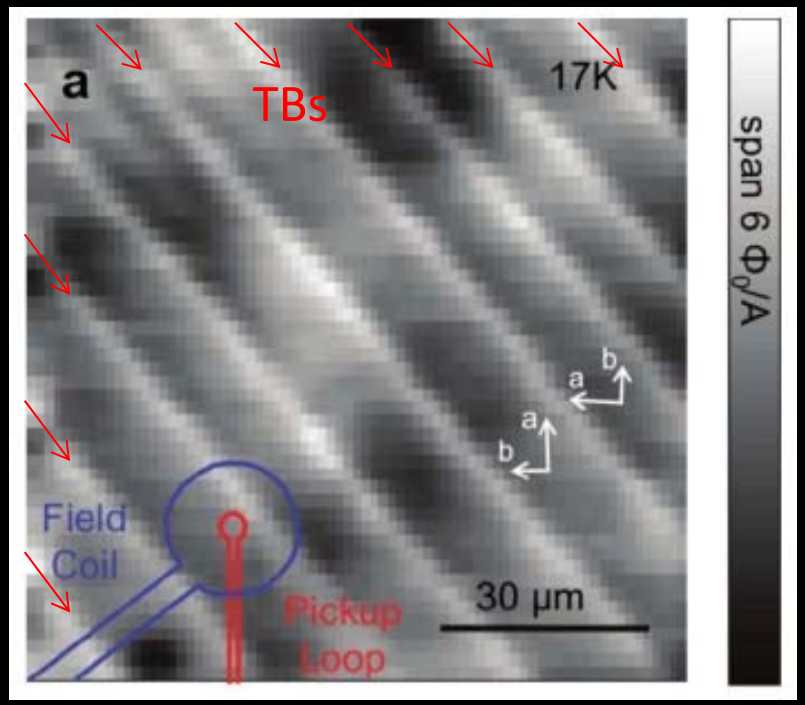
TBs also exist in 122 iron based superconductors!



Tanatar, PRB 79, 180508 (2009)

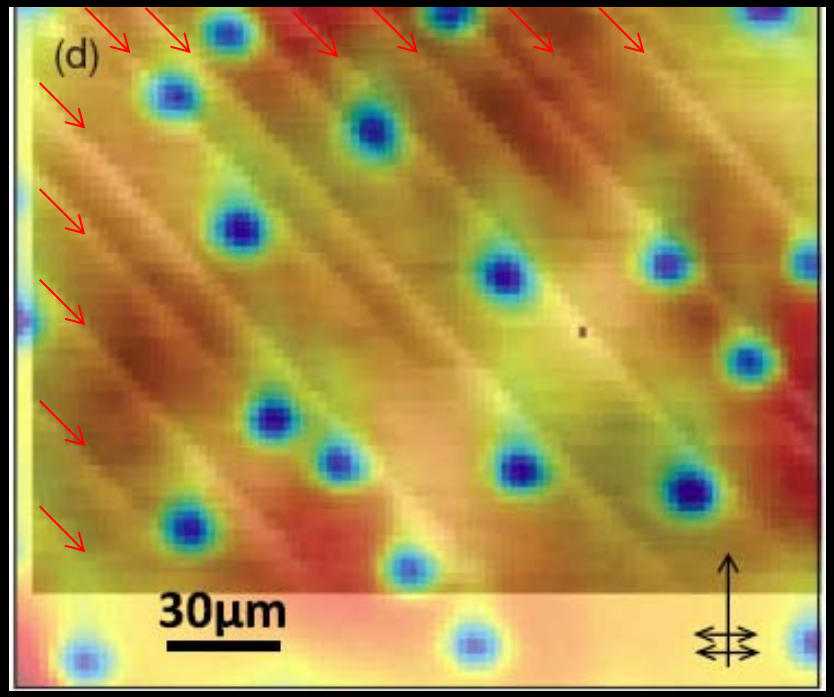
Twin boundaries in $Ba(Fe_{1-x}Co_x)_2As_2$

Susceptometry



Kalisky, PRB 81, 184513 (2010)

Magnetometry



Kalisky, PRB 83, 064511 (2011)

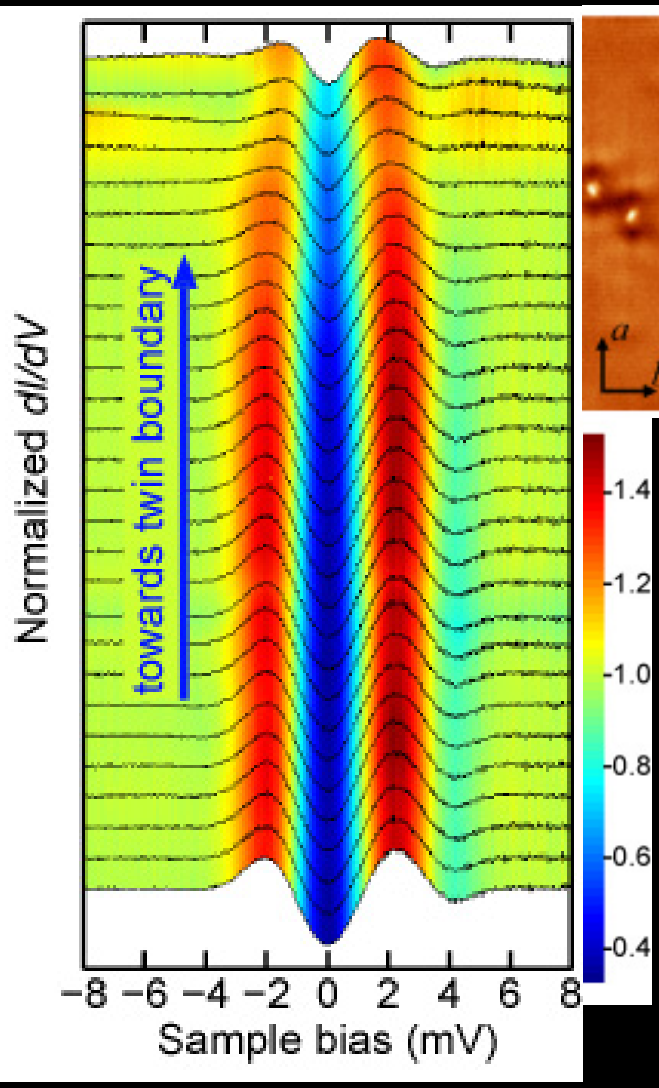
Enhanced superfluid density on TBs

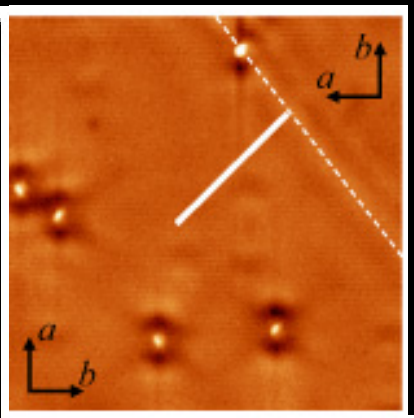
Vortices avoid TBs

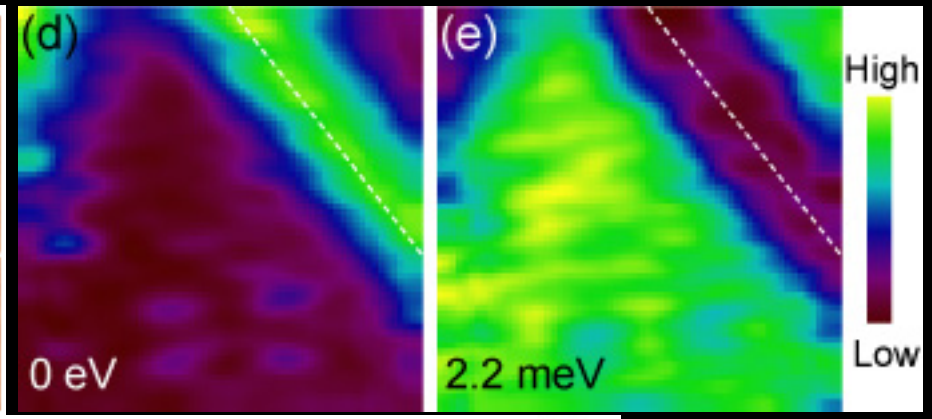
Why? doping? strain?

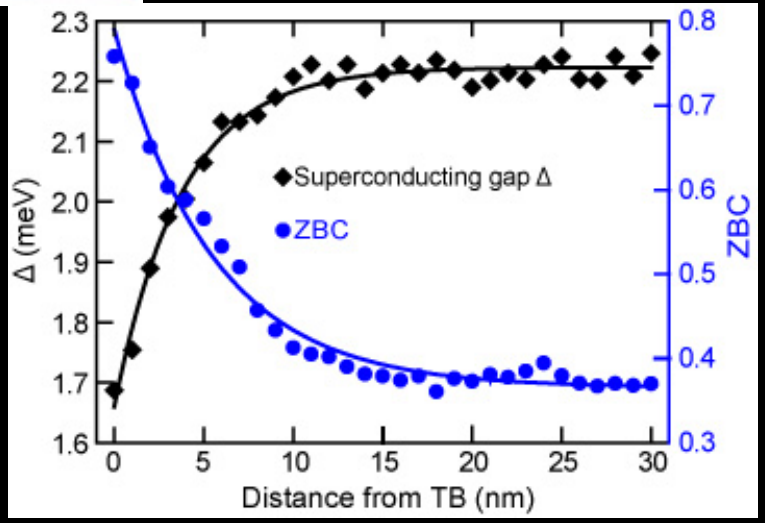
→ look at stoichiometric FeSe to eliminate possible doping variations

Twin boundaries in FeSe









ξ ~ 5.1 nm

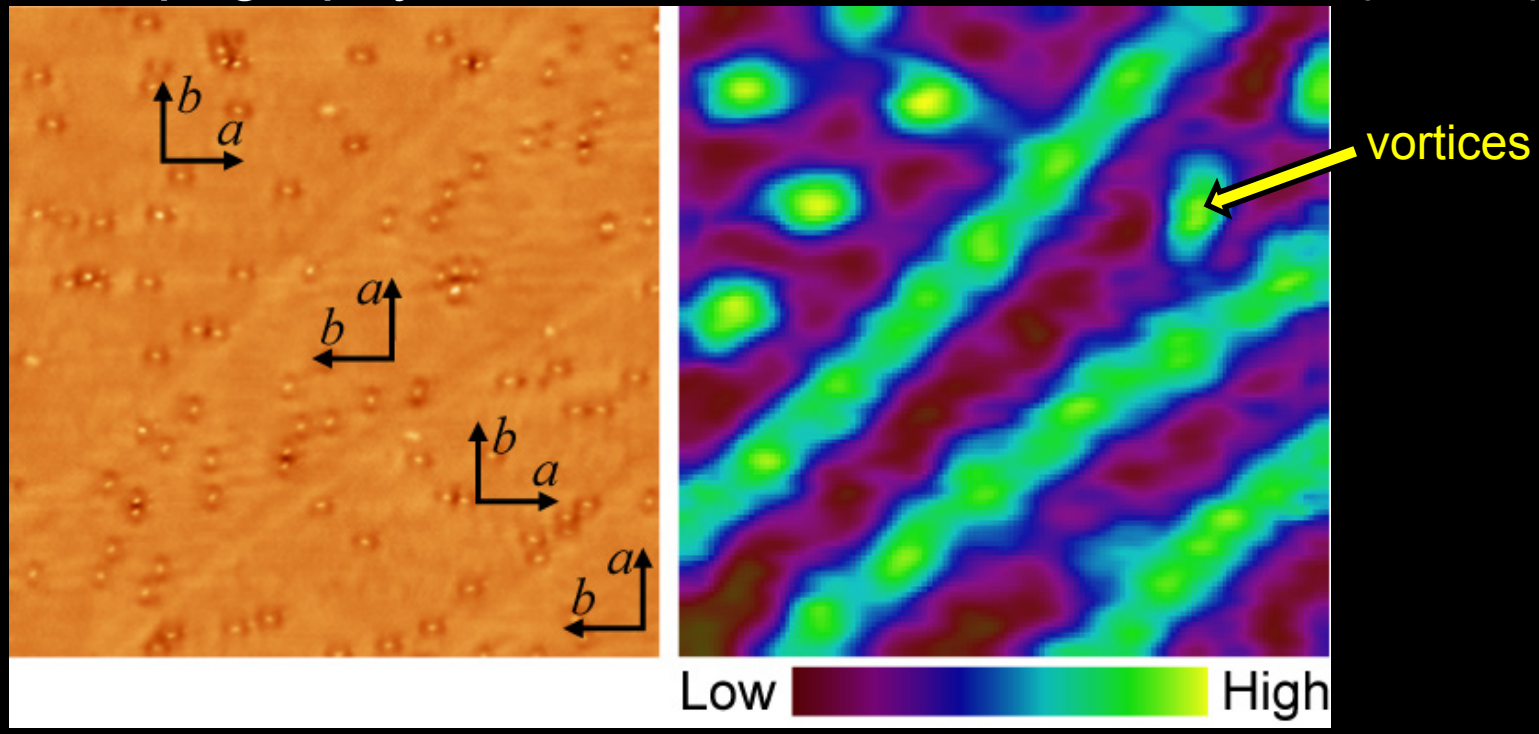
TBs suppress superconductivity in FeSe!

Song, PRL 109, 137004 (2012)

Vortex pinning at TBs in FeSe

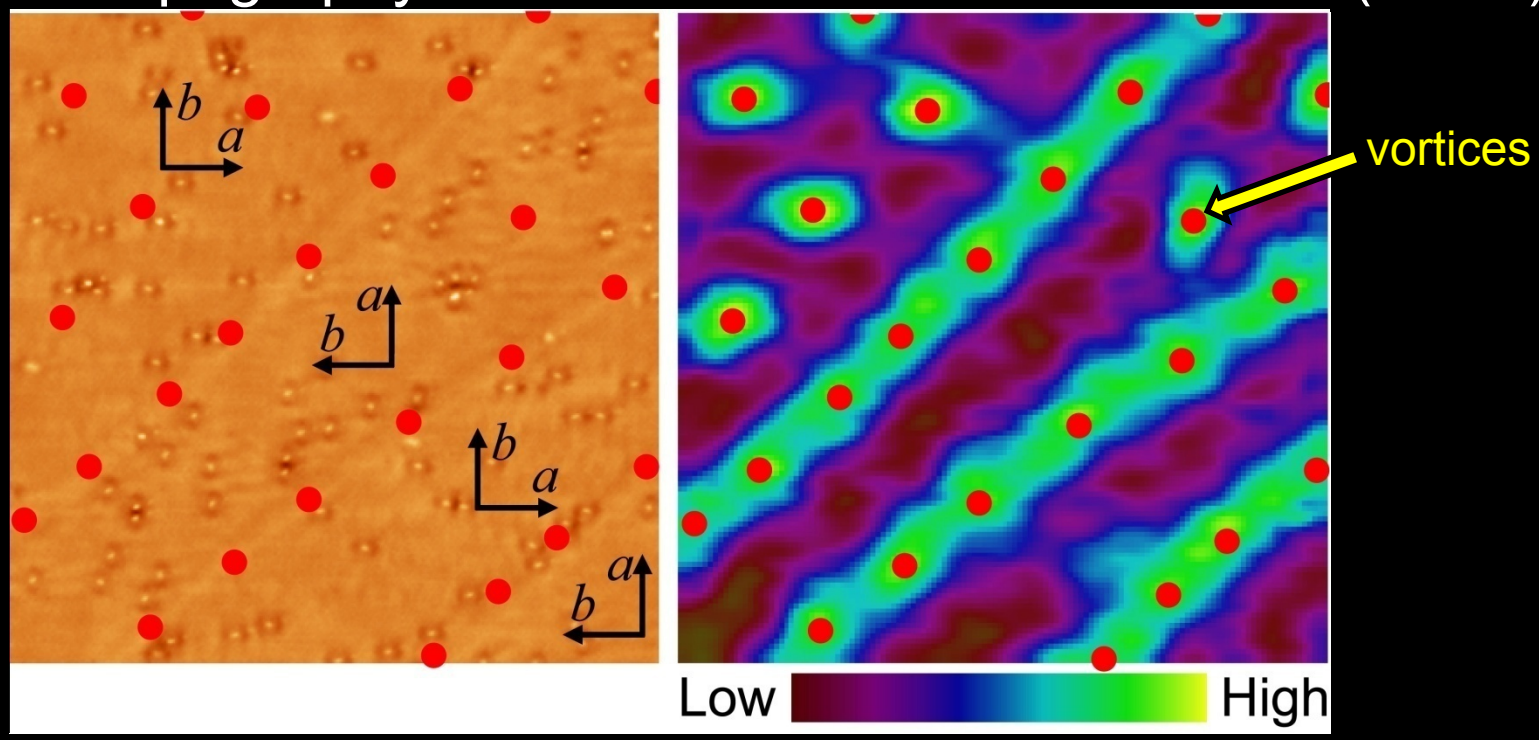
Topography

Zero bias conductance (B=2T)



Song, PRL 109, 137004 (2012)

Vortex pinning at TBs in FeSe



Consistency between vortex pinning and suppressed superconductivity at TBs.

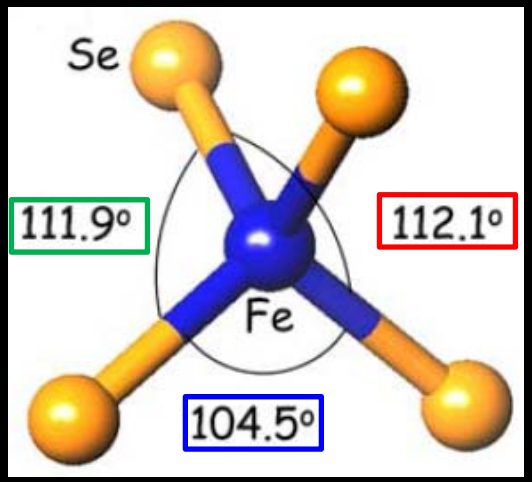
Song, PRL 109, 137004 (2012)

How does TB suppress superconductivity?

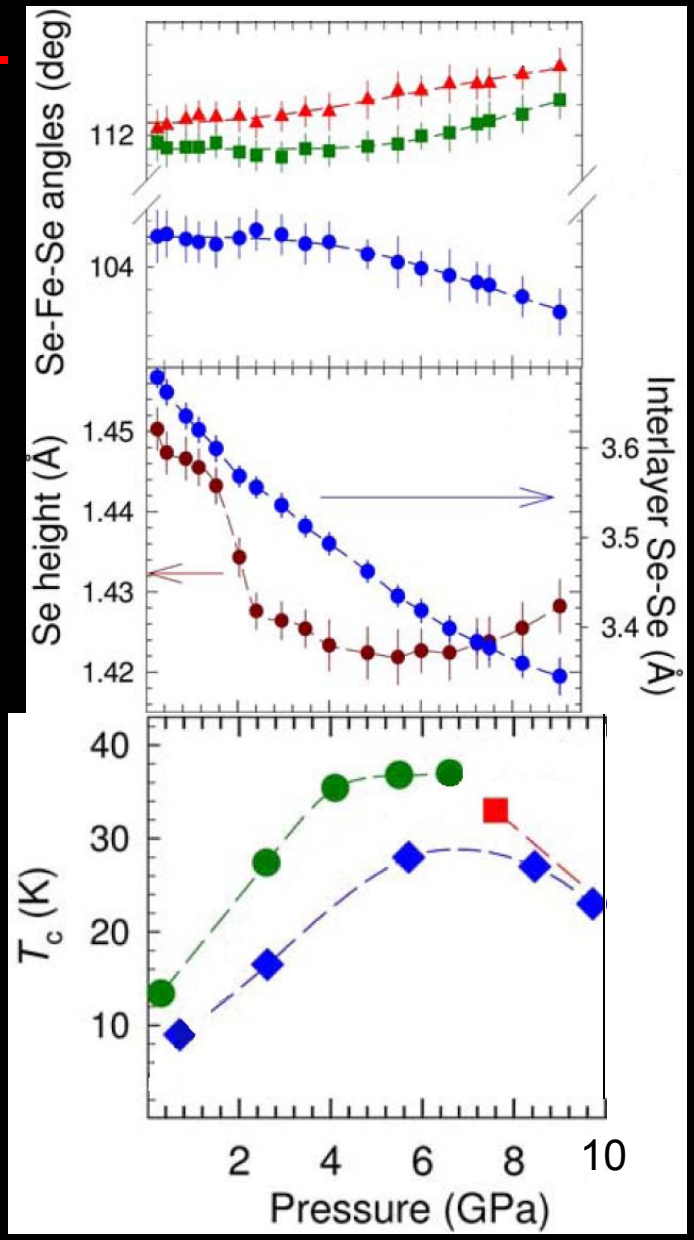
~~1. Variation in chemical doping across TB?~~

No, stoichiometric.

~~2. Tetrahedral angle?~~



No, α changes little with pressure, but T_c changes a lot.



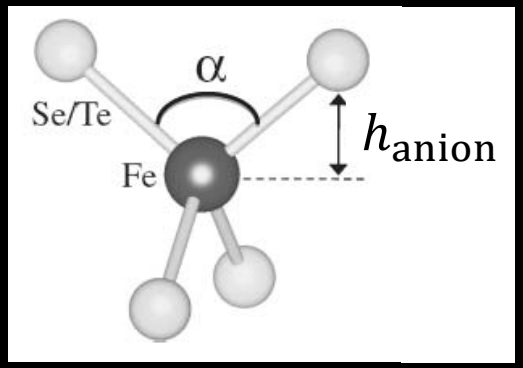
Margadonna, PRB 80, 064506 (2010)

How does TB suppress superconductivity?

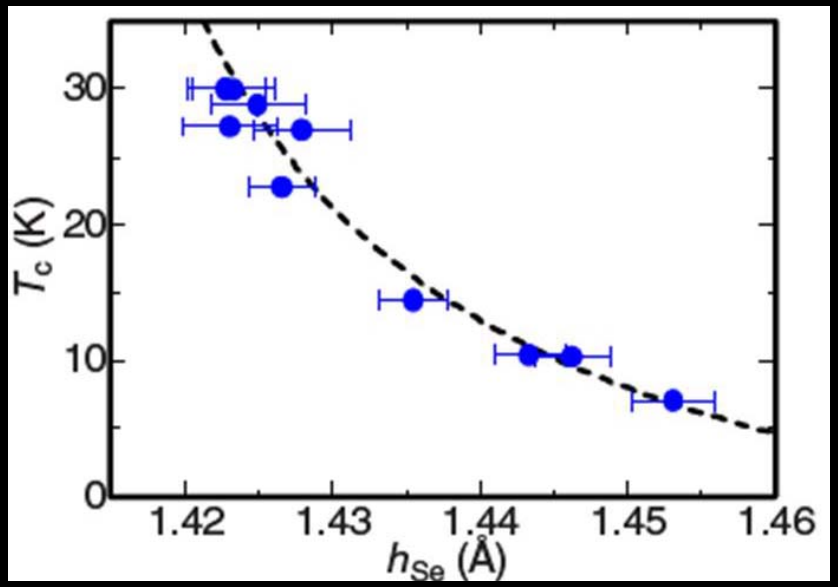
~~1. Variation in chemical doping across TB?~~

~~2. Tetrahedral angle?~~

3. h_{anion} (pnictogen or chalcogen) ?

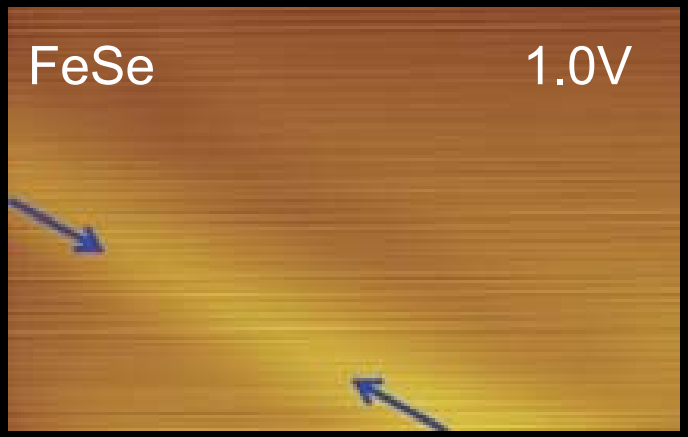


High-pressure measurements:



Okabe, PRB 81, 205119 (2010)

STM data:

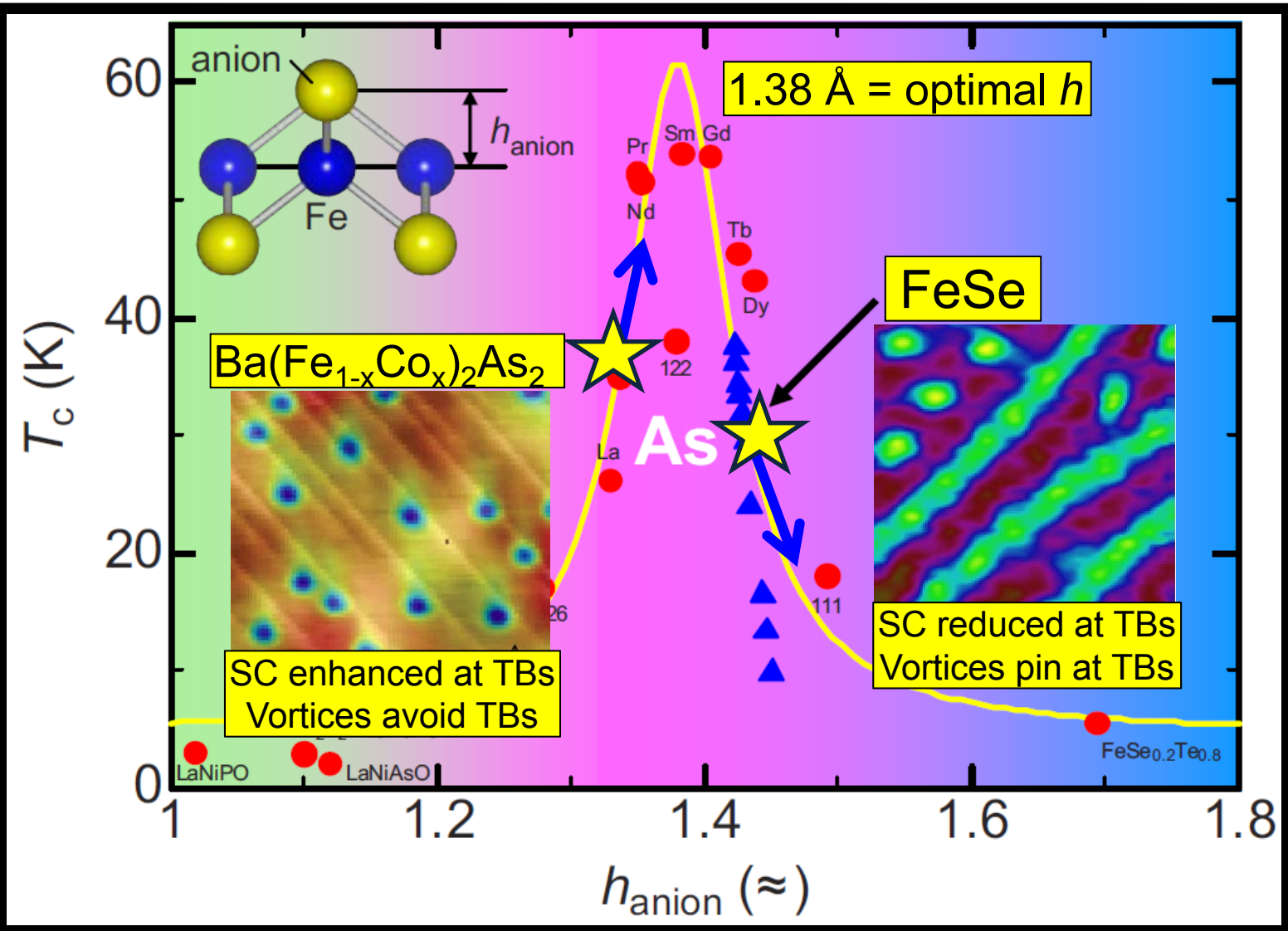


h_{Se} is enhanced on TB

Our hypothesis: TBs enhance the anion height.

Enhanced h_{Se} → reduced SC → vortices pin on TBs in FeSe

FeSe vs. $Ba(Fe_{1-x}Co_x)_2As_2$



Okabe, PRB 81, 205119 (2010)

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Outline

Boson mode

- seen in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$, LiFeAs, $NaFe_{1-x}Co_xAs$, and now FeSe
- $\Omega(r)$ correlates with $\Delta(r)$ in FeSe (*c.f.* anti-correlation in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$)

$$\Delta(r) = \Omega(r)\exp\left(\frac{-\Omega(r)}{2N_0 g^2}\right)$$

Twin boundaries

- repel vortices in $Ba(Fe_{1-x}Co_x)_2As_2$, but pin vortices in FeSe
- enhance pnictogen/chalcogen height?

Fe site defects

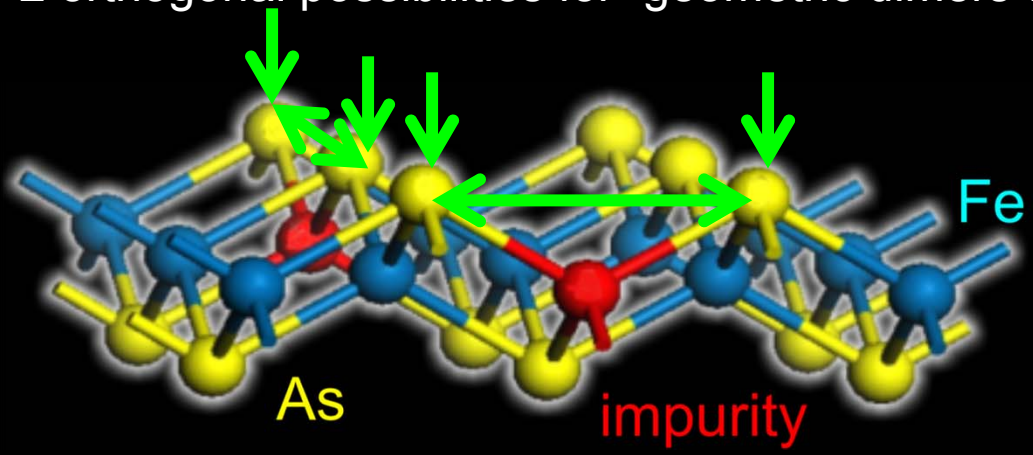
- geometric dimers
- electronic dimers cause transport anisotropy

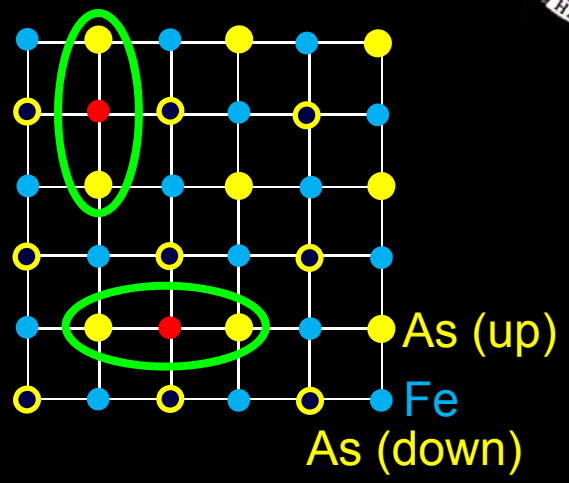
Vortices

- no anisotropy observed in $NdFeAsO_{1-x}F_x$
- single-vortex pinning force ~8 picoNewtons in $NdFeAsO_{1-x}F_x$
- $\lambda \sim 500\ \mathrm{nm}$ in $NdFeAsO_{1-x}F_x$

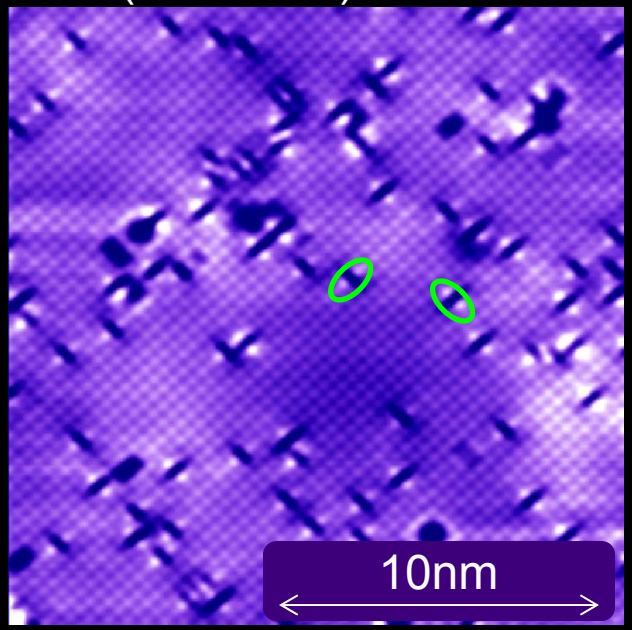
Fe-based SC survey: Impurities at Fe sites

2 orthogonal possibilities for "geometric dimers":



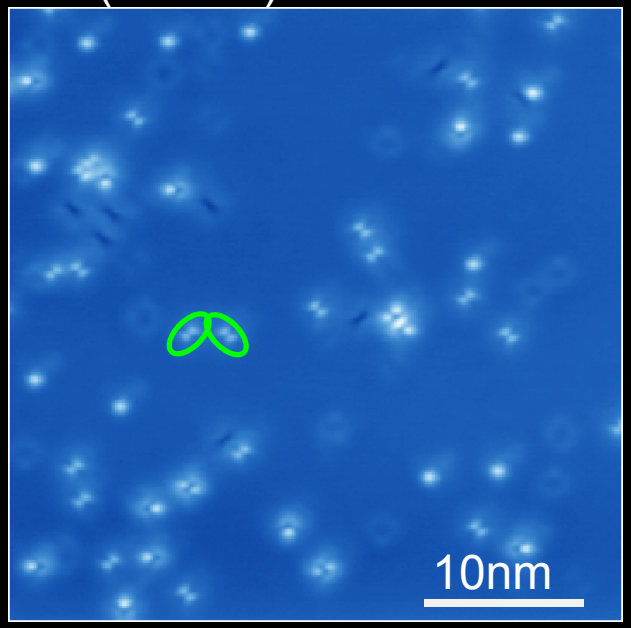


1111 (LaFeAsO)



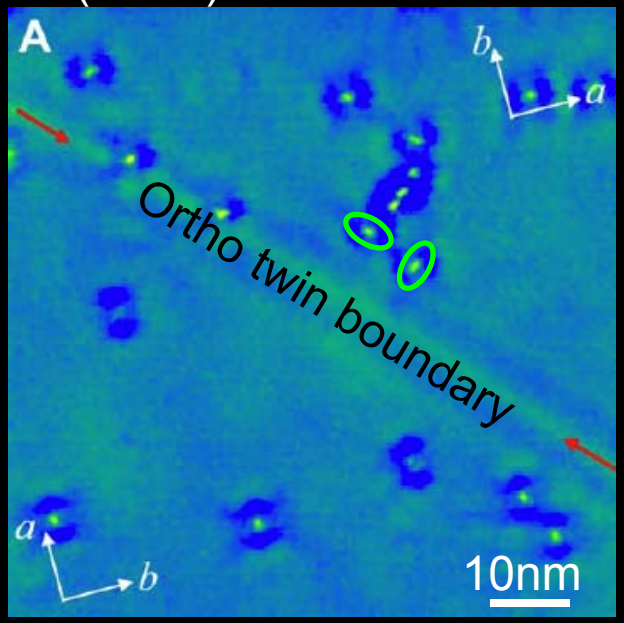
Zhou, PRL 106, 087001 (2011)

111 (LiFeAs)



Hanaguri, PRB 85, 214505 (2012)

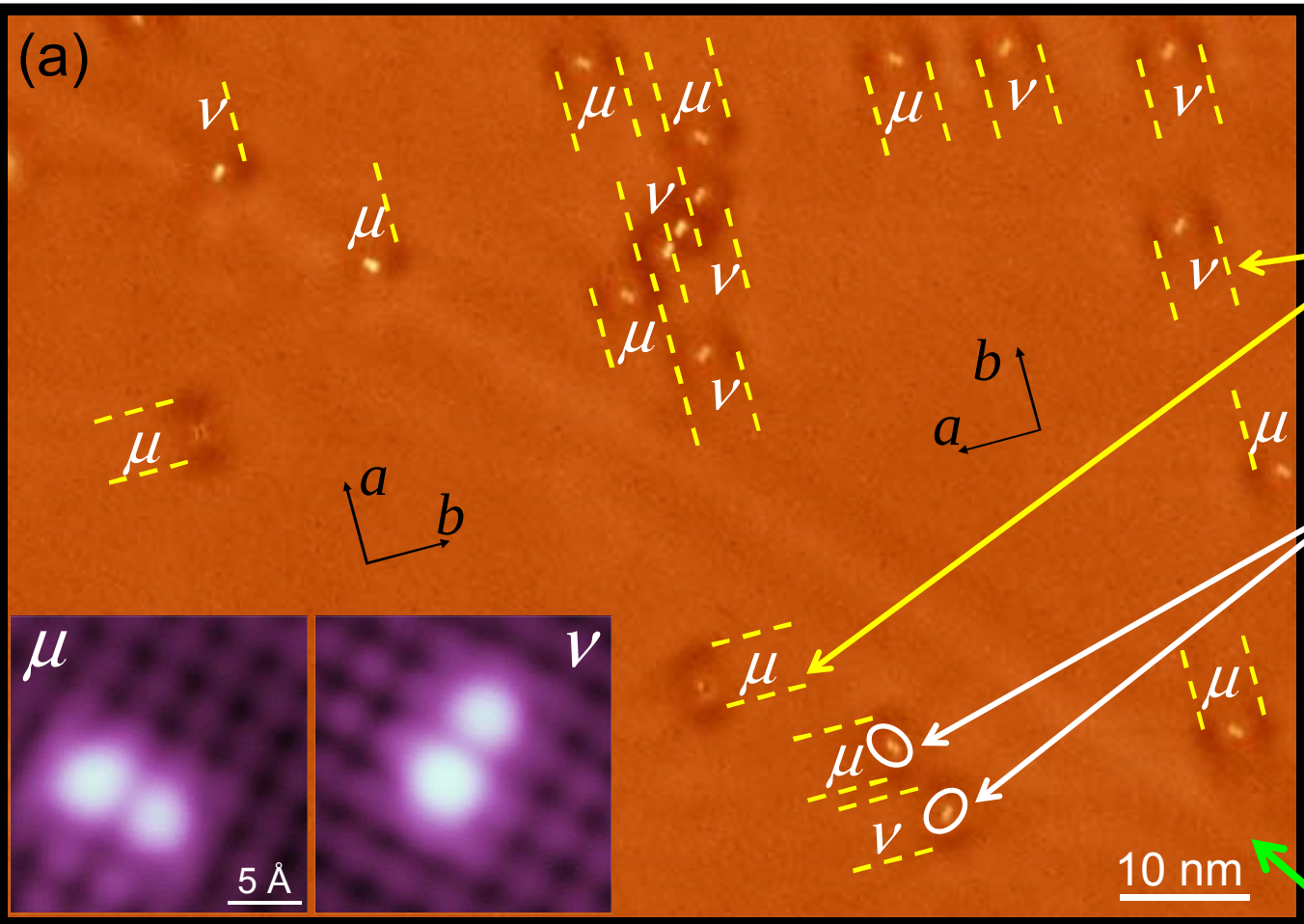
11 (FeSe)



Song, Science 332, 1410 (2011)

Common phenomenology → take a closer look at FeSe defects…

FeSe: Impurities at Fe sites



topography
V = 10 mV, I = 0.1 nA

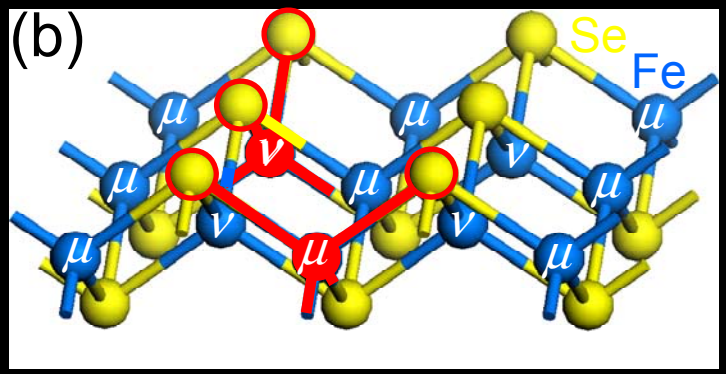
Electronic dimers: always along Fe-Fe, a-axis

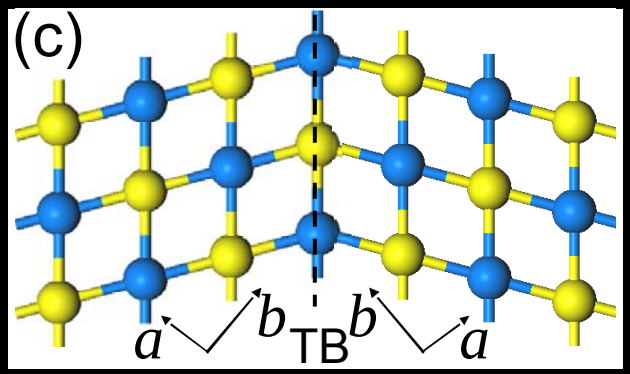
Exist only for E within ±20 meV → purely electronic

Geometric dimers μ and ν, randomly oriented, 45° to a & b axes

Exist over large energy range

orthorhombic twin boundary

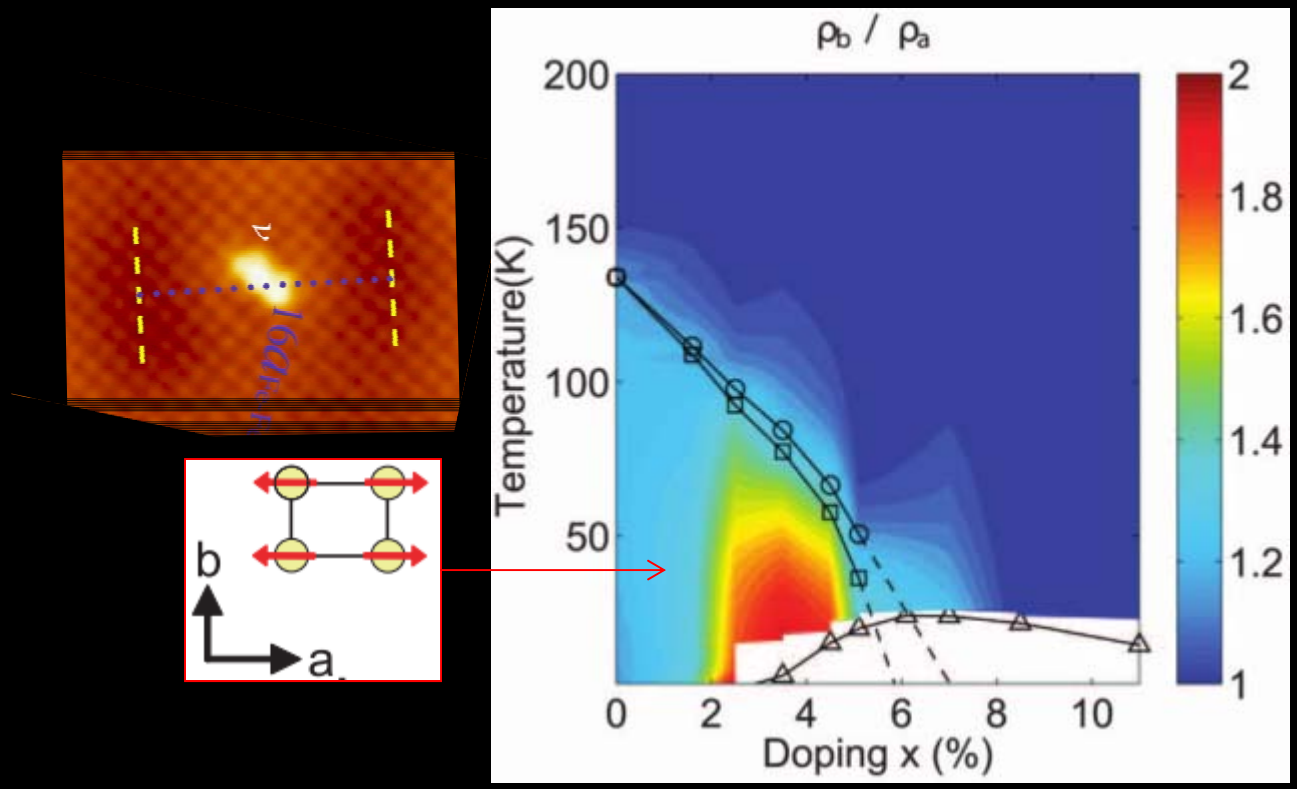




Song, PRL 109, 137004 (2012)

Transport anisotropy: Impurities at Fe sites?

$Ba(Fe_{1-x}Co_x)_2As_2$



Chu, Science 329, 824 (2010)

Transport observations:

1. Nematicity proportional to doping (but cuts off at ortho→tet transition)
2. Highest resistivity along *b* axis

Can these observations be related to the electronic dimers at the Fe site?

Transport anisotropy: Co dopants themselves?

Power spectrum of scattering:

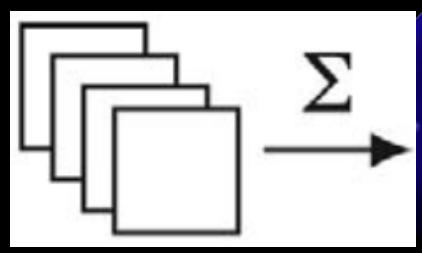
$$P(\mathbf{q},E) = \frac{1}{N}\left|\frac{1}{\pi}\mathrm{Im}\Lambda(\mathbf{q},E)\right|^2 |\delta\varepsilon(\mathbf{q})|^2$$

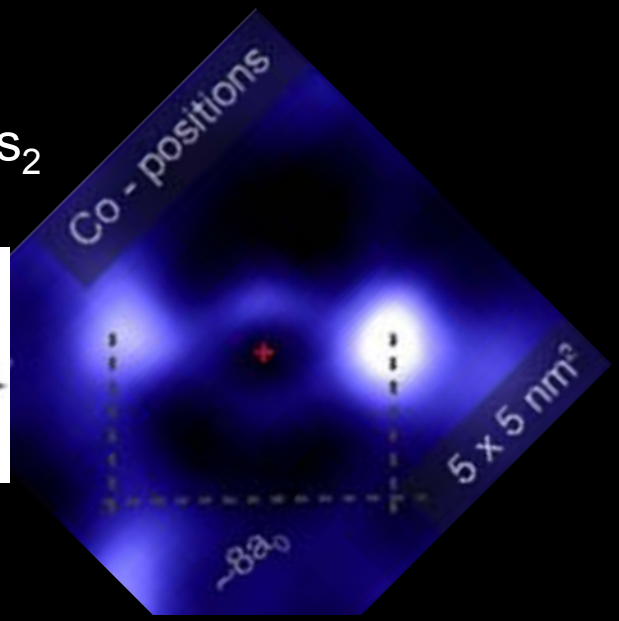
'bare' QPI from point scatterer:

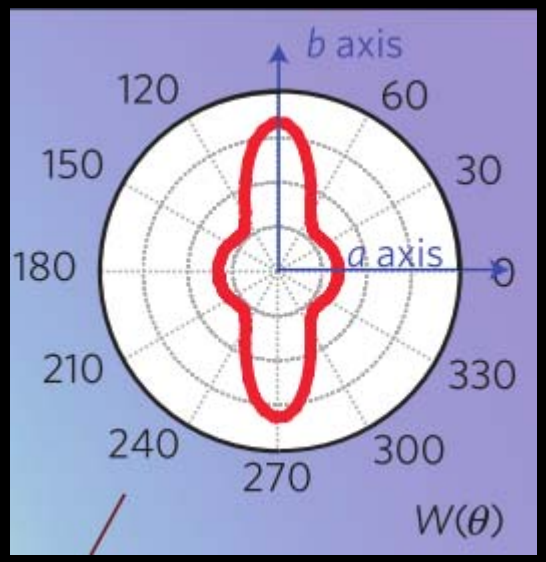
$$\Lambda(\mathbf{q},E) \equiv \int \mathrm{d}^2 r \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} G(\mathbf{r},E)G(-\mathbf{r},E)$$

structure factor of the scatterer (Fourier transform of the r-space scattering potential)

$Ca(Fe_{1-x}Co_x)_2As_2$







Allan, Nat Phys 9, 220 (2013)

Conclusion: yes! the Fe site impurities can cause transport anisotropy!

Outline

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- $\Omega(r)$ correlates with $\Delta(r)$ in FeSe (*c.f.* anti-correlation in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$)

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- no anisotropy observed in $NdFeAsO_{1-x}F_x$
- single-vortex pinning force ~8 picoNewtons in $NdFeAsO_{1-x}F_x$
- $\lambda \sim 500\ \mathrm{nm}$ in $NdFeAsO_{1-x}F_x$

Vortex Pinning Motivation

Understand vortex pinning in Fe-based superconductors
at the single vortex level

Technology:

- Vortex motion inhibits critical current J_c → need to enhance pinning
- understand the impact of individual pinning defects

Physics:

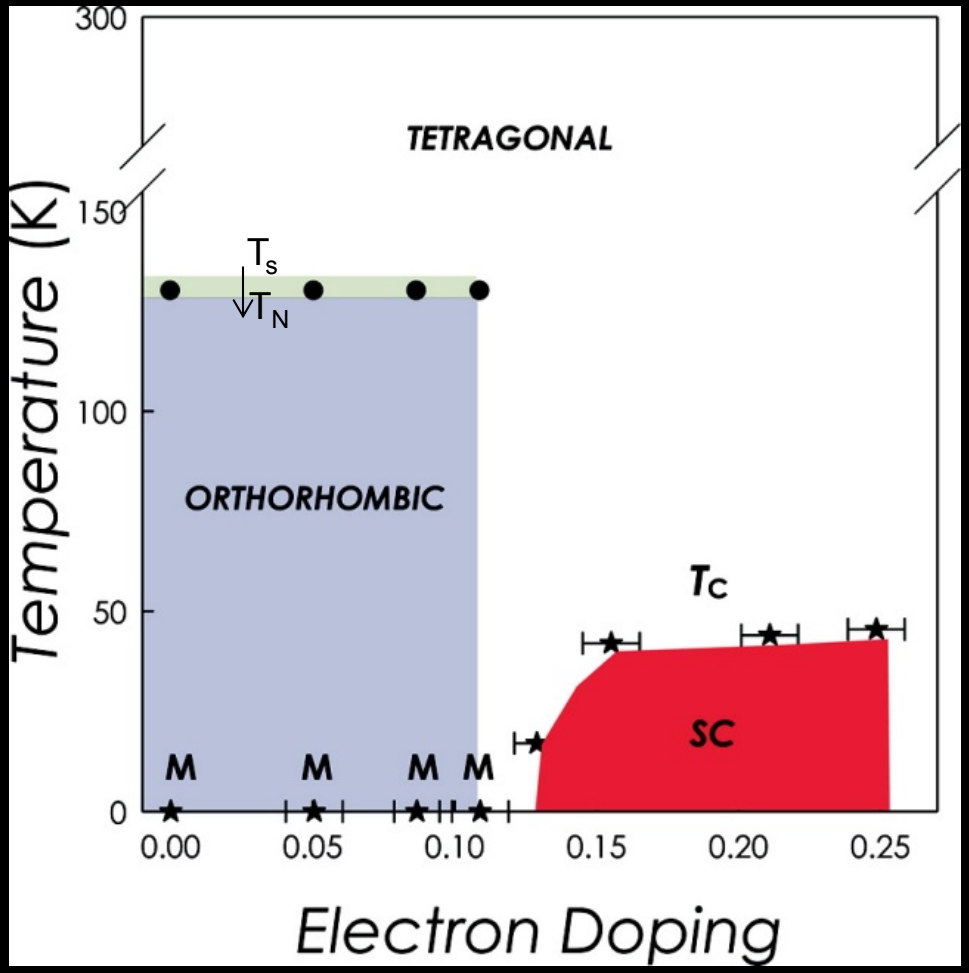
- vortex elasticity → electronic anisotropy
- anisotropic pinning → vortex core shape

  → gap symmetry? (anisotropic s, nodal d?)

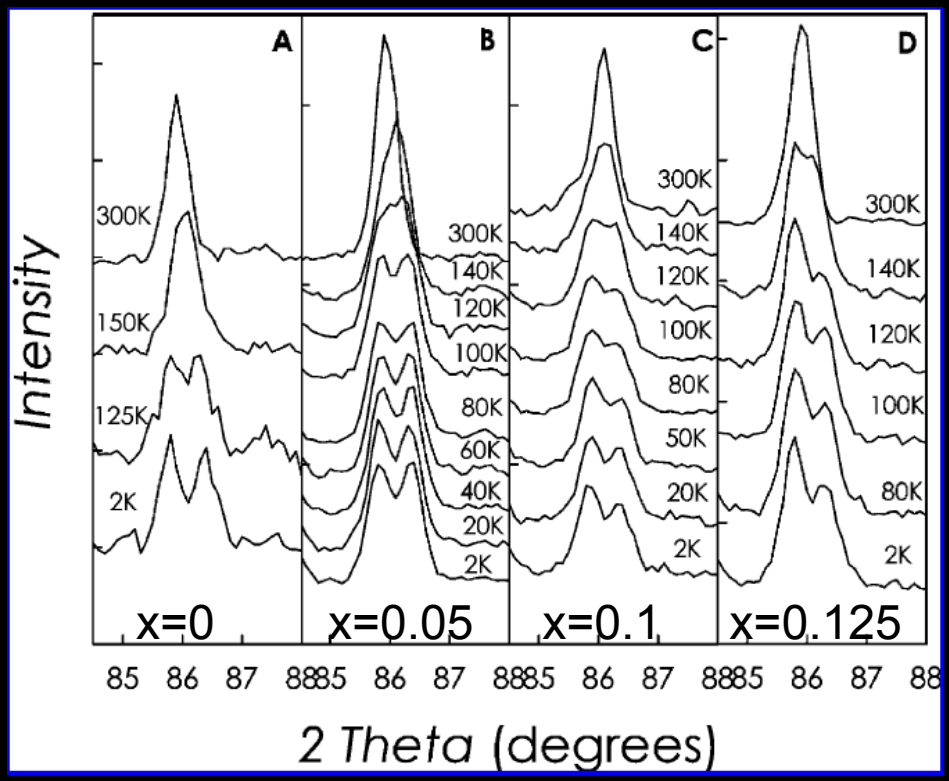
→ study $NdFeAsO_{0.9}F_{0.1}$ because it has high T_c ~ 50K

→ use local tool, magnetic force microscopy, to access single vortices

$NdFeAsO_{1-x}F_x$



Neutron diffraction data:

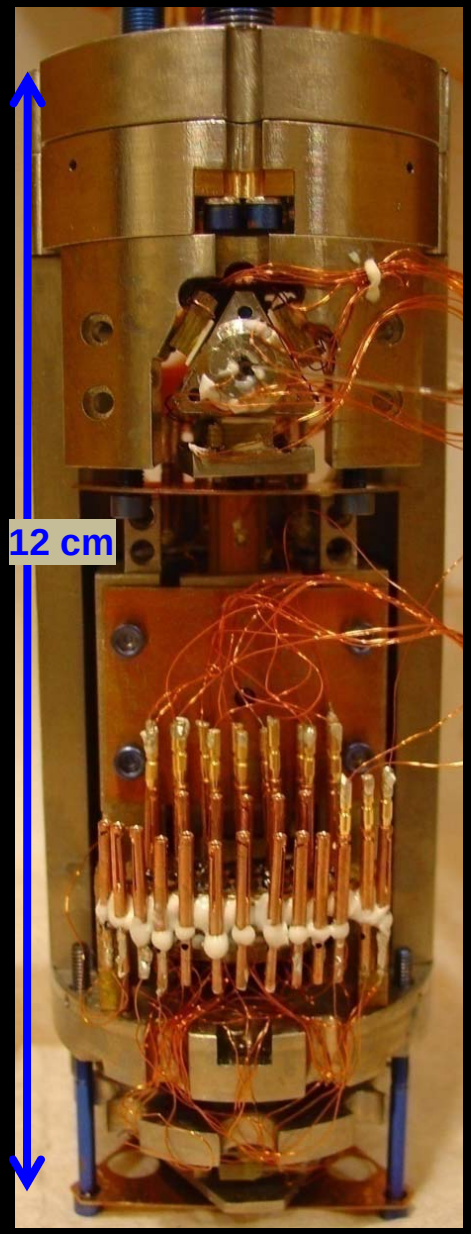


"Only for these four samples (x=0, 0.05, 0.10, and 0.125) was it possible to observe a clear splitting of the tetragonal (220) Bragg reflection into the (040) and (400) orthorhombic reflection."

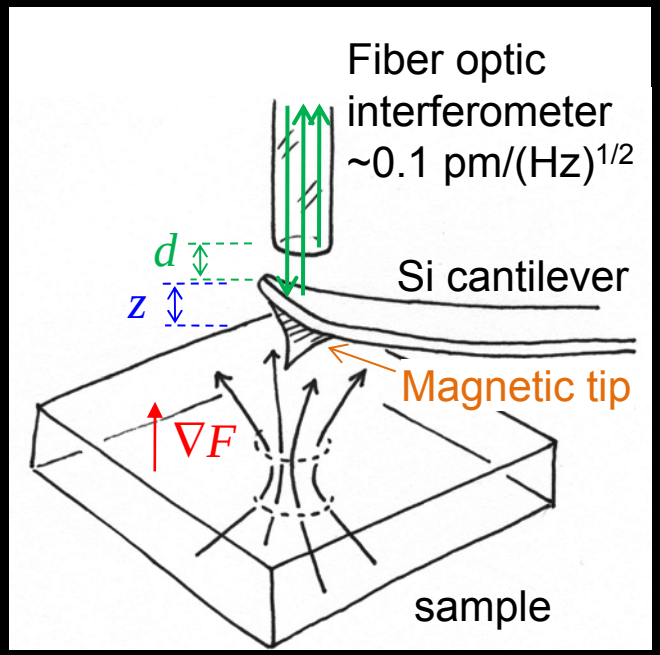
It doesn't say that there is no ortho transition for higher x, just says that it was not possible to observe clear splitting.

Malavasi, JACS 132, 2417 (2010)

Magnetic Force Microscope



built by Dr. Jeehoon Kim



Tip-sample force:

$$\mathbf{F} = \nabla(\mathbf{m} \cdot \mathbf{B})$$

Frequency modulation imaging (measures force gradient):

$$\frac{\Delta f}{f_0} = -\frac{1}{2k}\frac{dF_z}{dz}$$

Pros and Cons of MFM

Tip Geometry
Con: Imperfectly known
Pro: Up to 20 nm spatial resolution

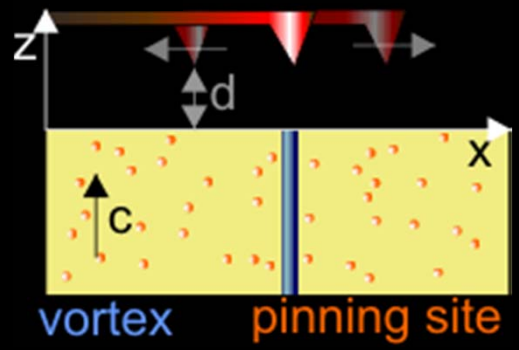
Other signals
Con: See atomic forces too
Pro: Simultaneous topography

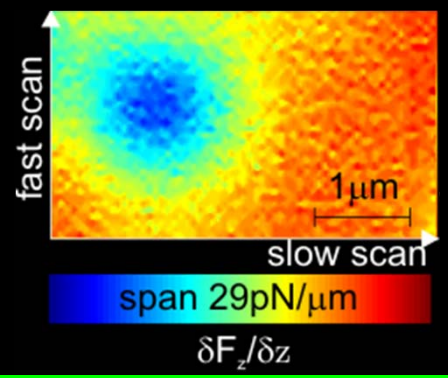
Invasiveness
Con: Tip exerts force on vortex
Pro: Tip exerts force on vortex

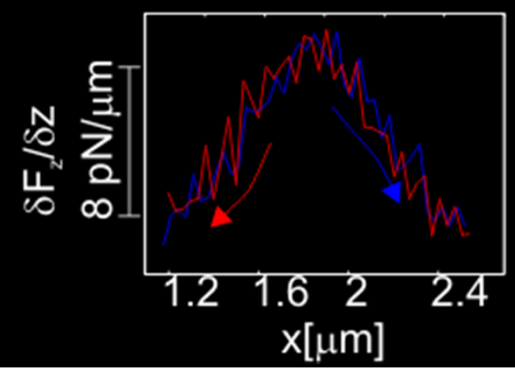
Vertical force gradient → imaging
Horizontal force → manipulation

Vortex Manipulation in $NdO_{1-x}F_xFeAs$

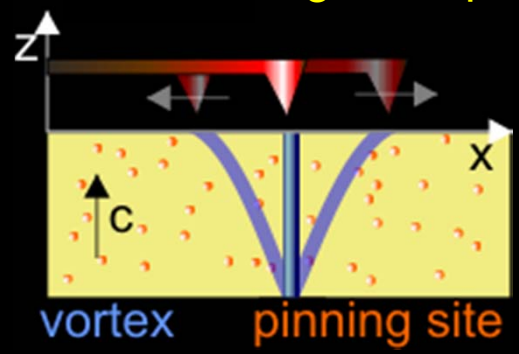
d large (tip far from sample, small force): image without disturbing vortex

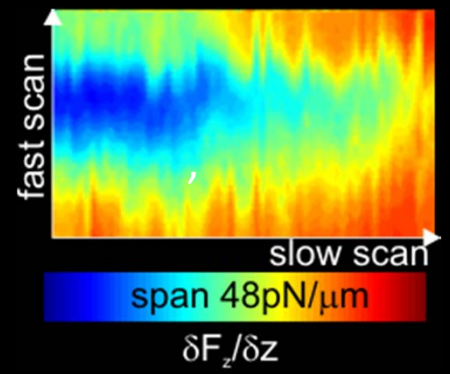


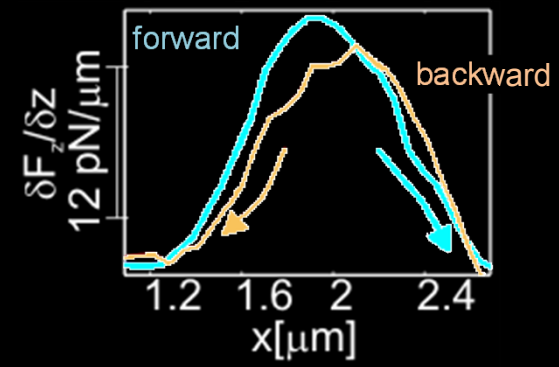




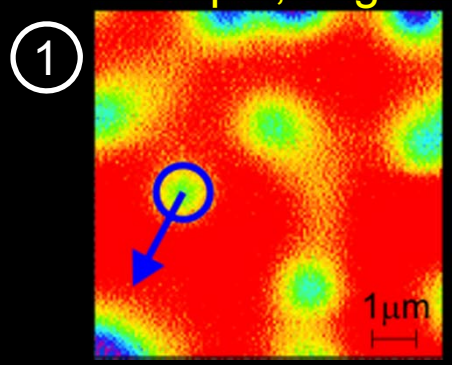
d intermediate: drag the top of the vortex

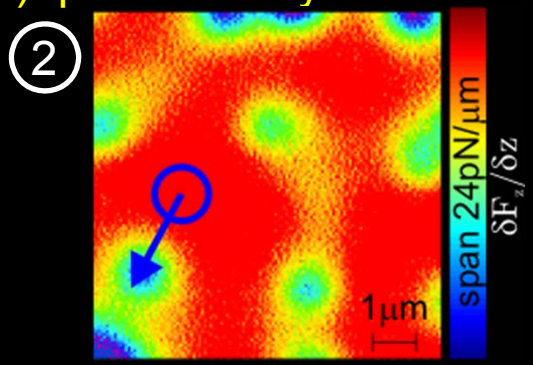


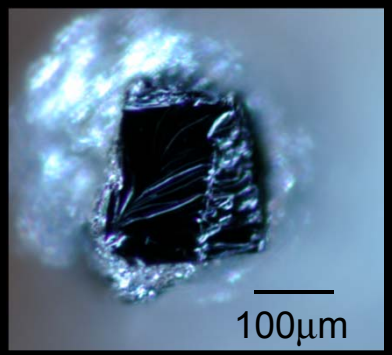




d small (tip close to sample, large force): permanently move the entire vortex

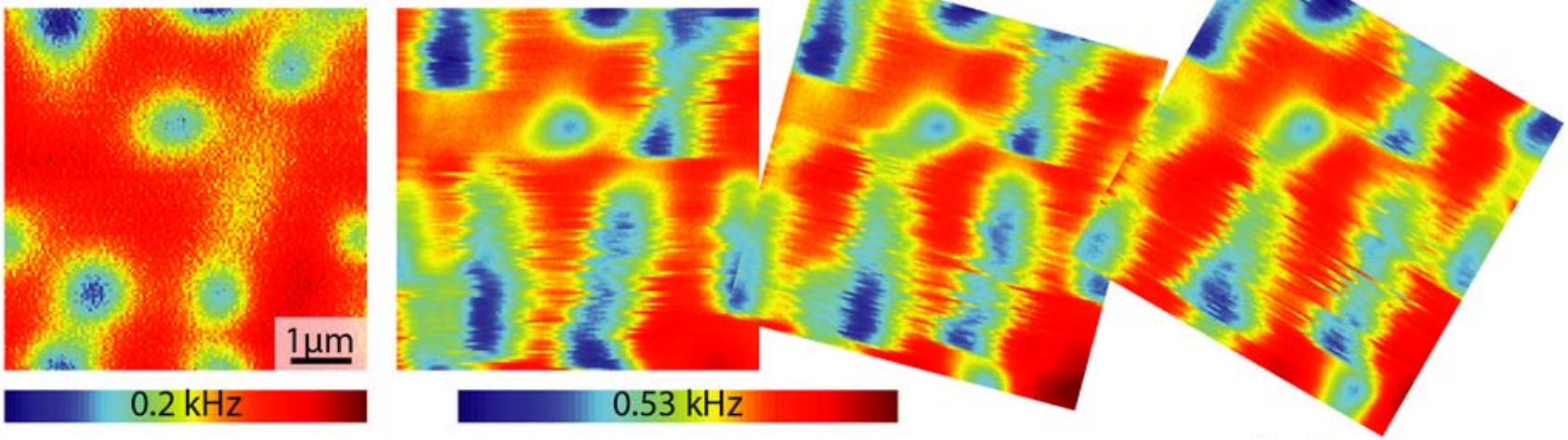


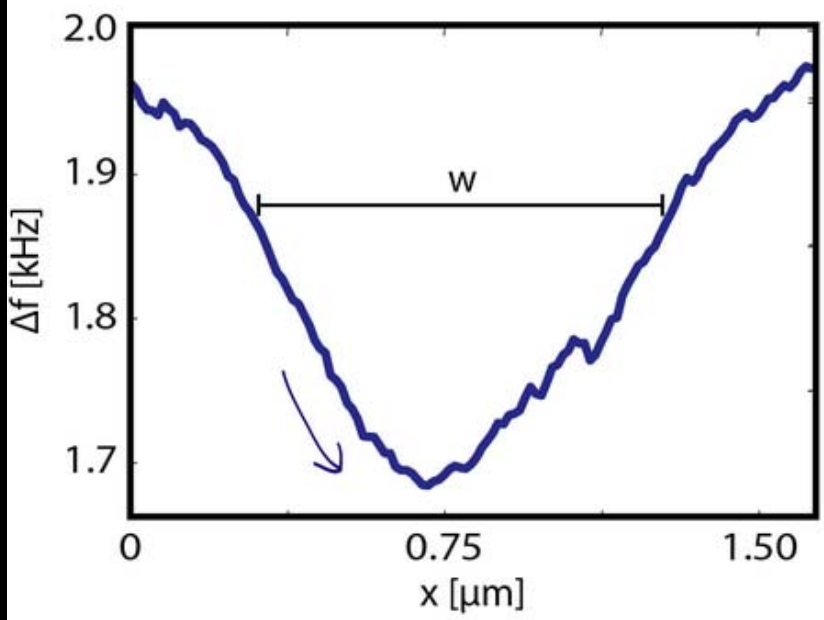


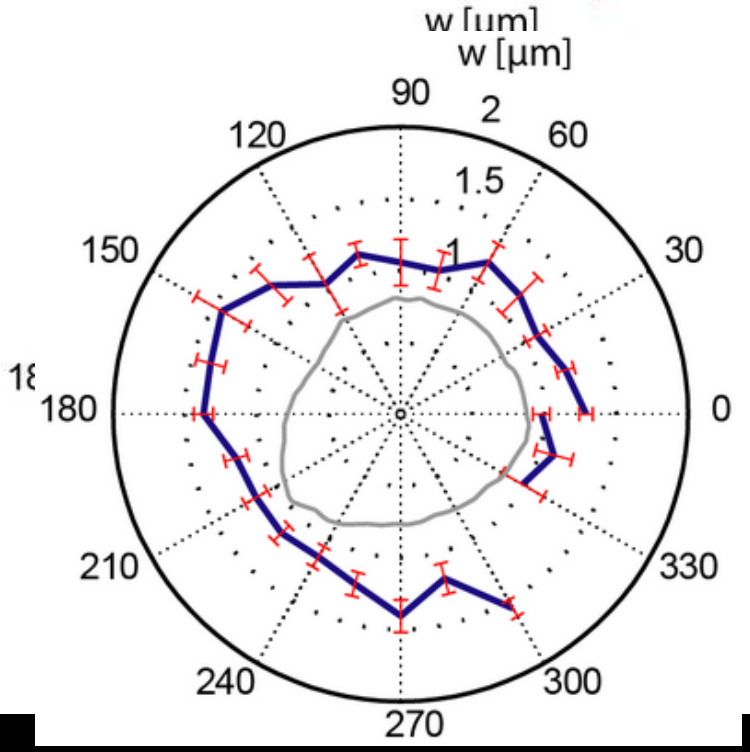


Angular dependence in $NdO_{1-x}F_xFeAs$

d intermediate: drag the top of the vortex



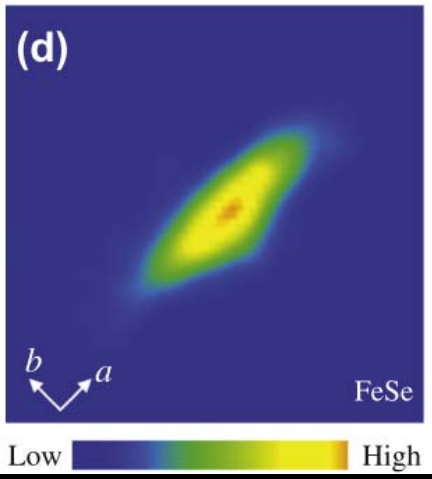




Vortex anisotropy ?

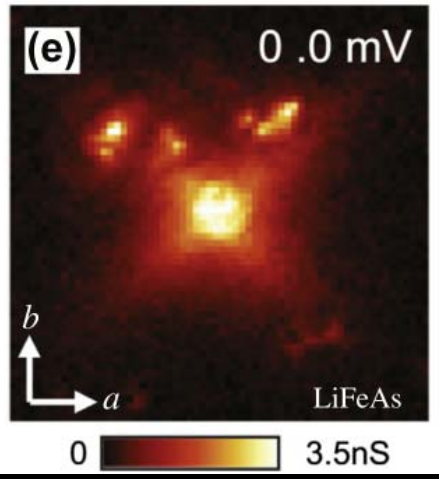
STM

FeSe



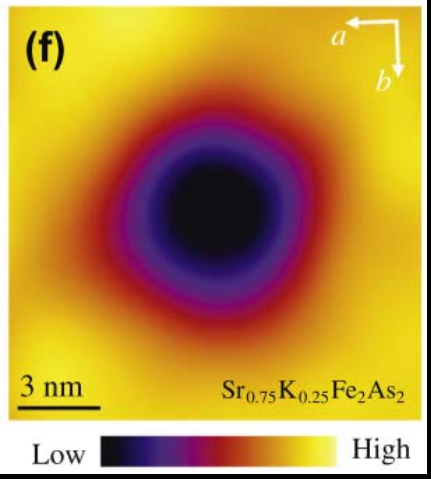
Song, Science (2011)

LiFeAs



Hanaguri, PRB (2012)

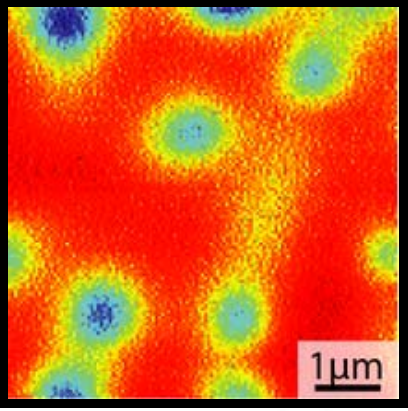
$Sr_{1-x}K_xFe_2As_2$

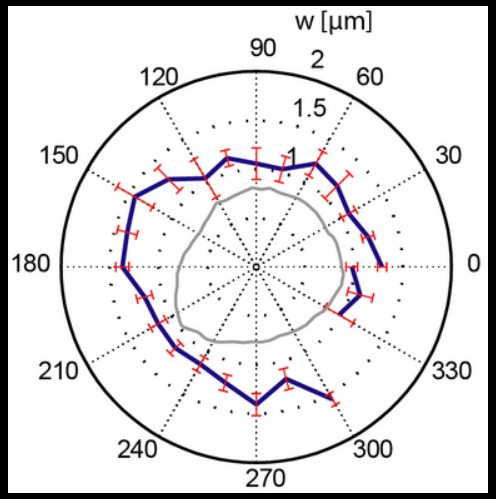


Song, PRB (2013)

MFM

$NdFeAsO_{1-x}F_x$

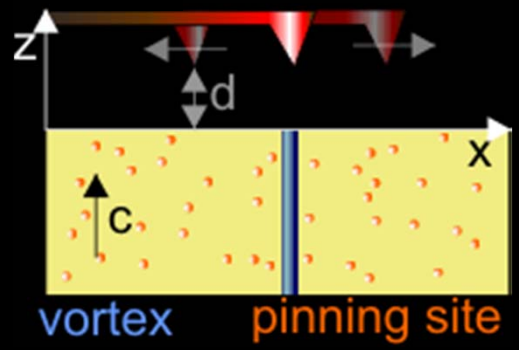


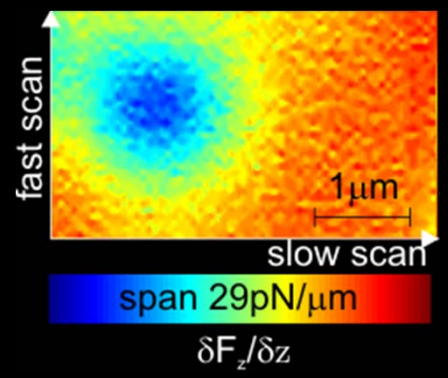


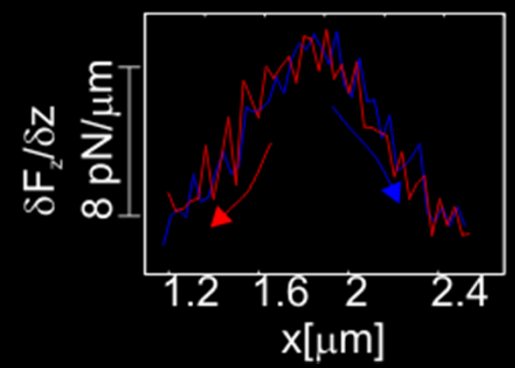
Jessie Zhang
(to be submitted)

Vortex Manipulation in $NdO_{1-x}F_xFeAs$

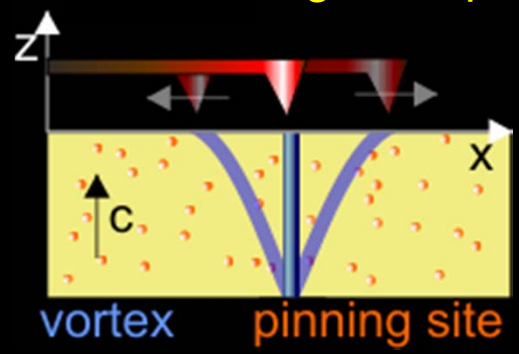
d large (tip far from sample, small force): image without disturbing vortex

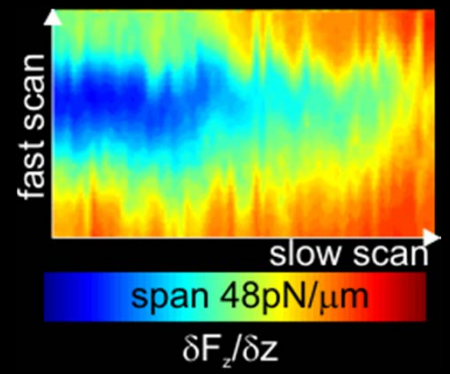


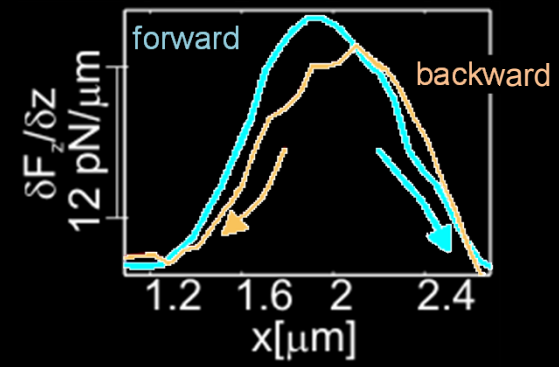




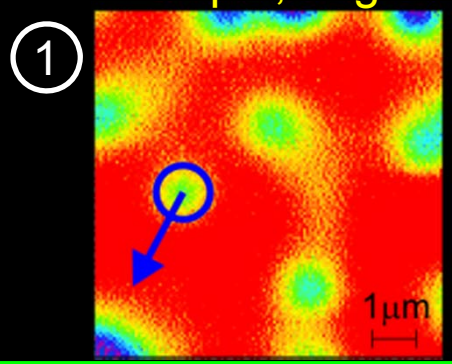
d intermediate: drag the top of the vortex

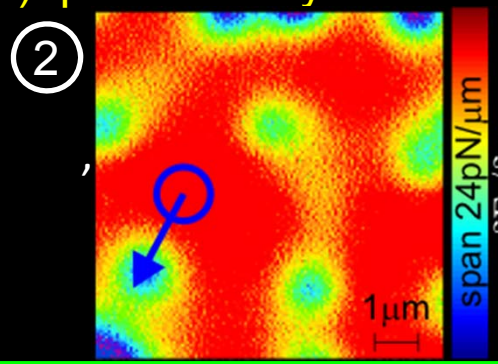


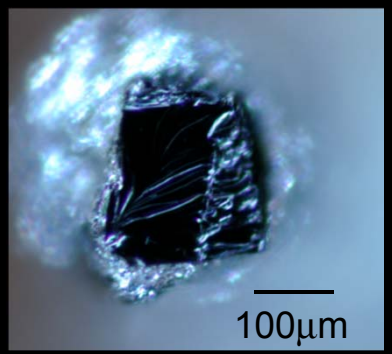




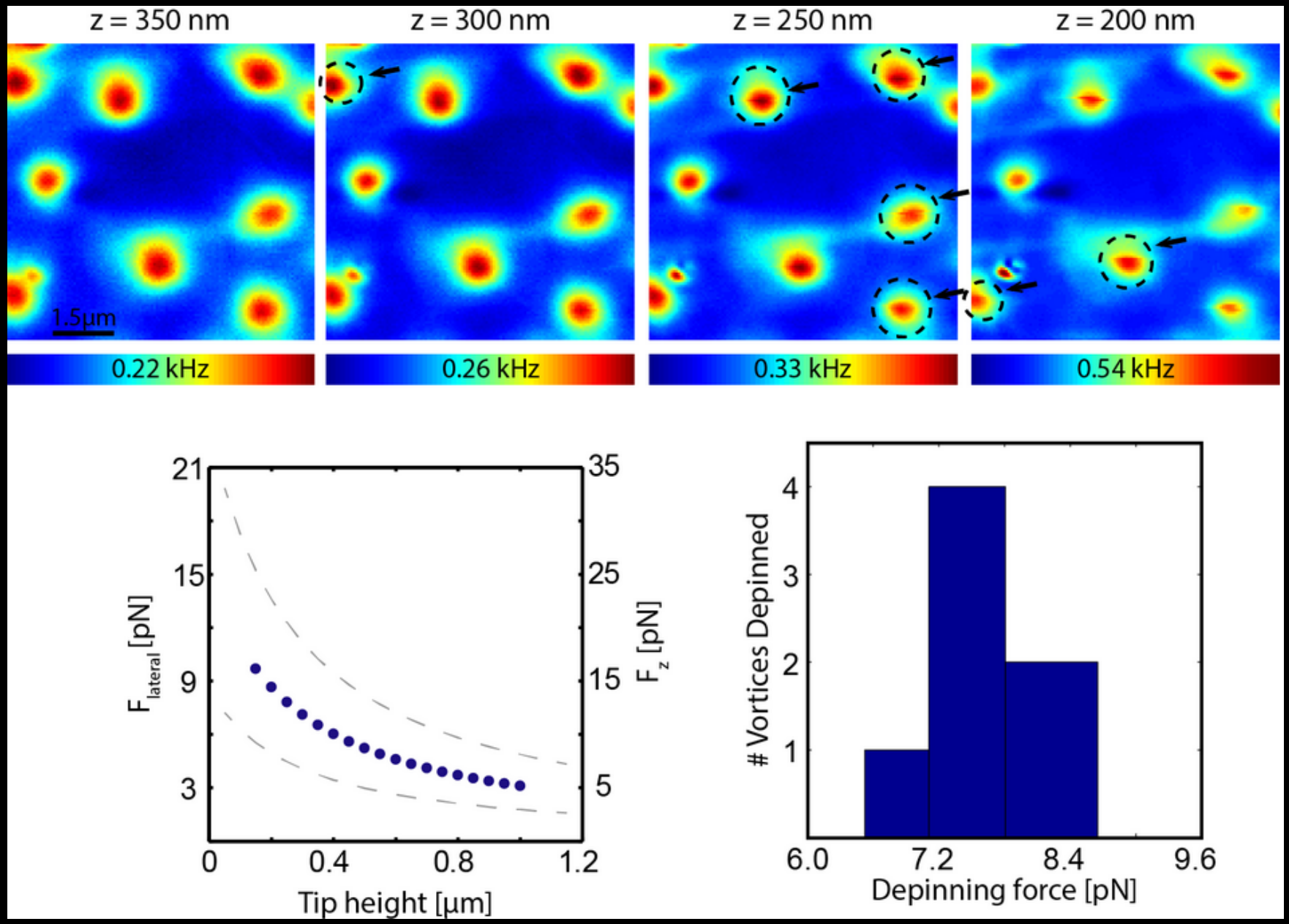
d small (tip close to sample, large force): permanently move the entire vortex





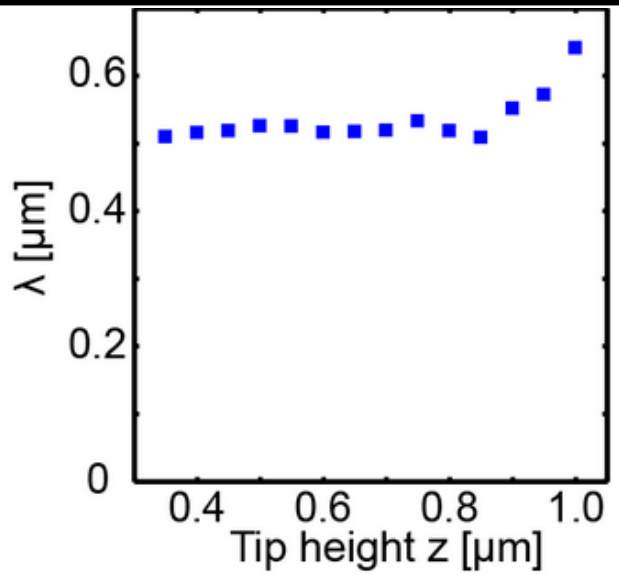


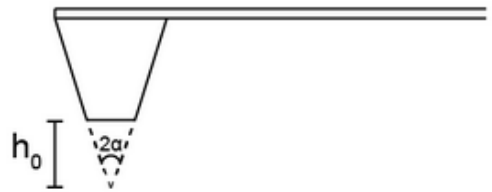
Vortex pinning force in $NdFeAsO_{1-x}F_x$



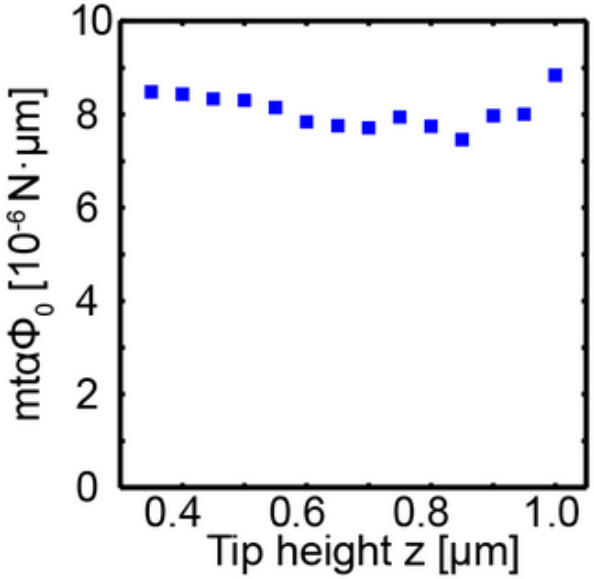
Jessie Zhang (to be submitted)

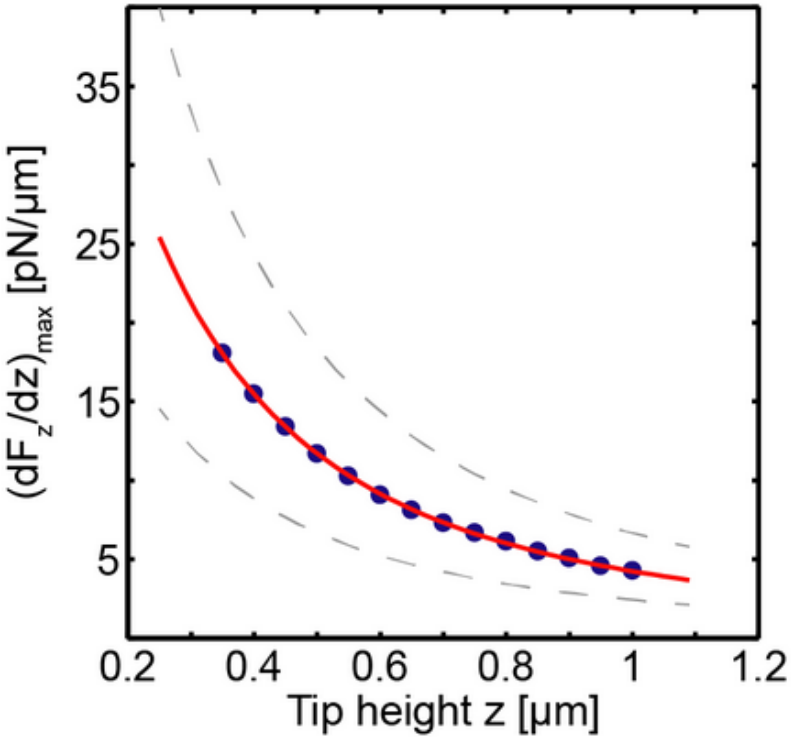
λ in $NdFeAsO_{1-x}F_x$





$$\max\left(\frac{dF_z}{dz}(z)\right) = m\Phi_0 t\alpha\left(\frac{1}{(z+\lambda)^2} + \frac{2h_0}{(z+\lambda)^3}\right)$$





Jessie Zhang (to be submitted)

Conclusions

Boson mode

- seen in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$, LiFeAs, $NaFe_{1-x}Co_xAs$, and now FeSe
- $\Omega(r)$ correlates with $\Delta(r)$ in FeSe (*c.f.* anti-correlation in $SmFeAsO_{1-x}F_x$, $K_xBa_{1-x}Fe_2As_2$)

$$\Delta(r) = \Omega(r)\exp\left(\frac{-\Omega(r)}{2N_0 g^2}\right)$$

Twin boundaries

- repel vortices in $Ba(Fe_{1-x}Co_x)_2As_2$, but pin vortices in FeSe
- enhance pnictogen/chalcogen height?

Fe site defects

- geometric dimers
- electronic dimers cause transport anisotropy

Vortices

- no anisotropy observed in $NdFeAsO_{1-x}F_x$
- single-vortex pinning force ~8 picoNewtons in $NdFeAsO_{1-x}F_x$
- $\lambda \sim 500\ \mathrm{nm}$ in $NdFeAsO_{1-x}F_x$

More work remains to understand $\Omega(r)$ and $g(r)$ vs. $\Delta(r)$!