

# Anisotropy of magnetic response in high-temperature superconductors

# Anisotropy of magnetic response in high-temperature superconductors

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# «Conventional» superconductors:

*model (theory) BCS*

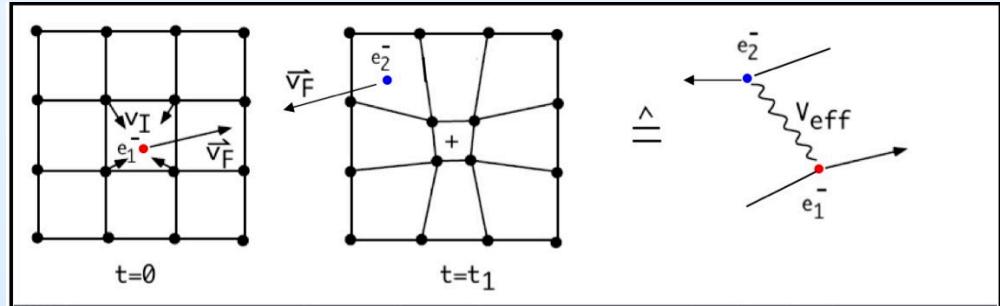
1957: J.Bardeen, L.Cooper, R.Schrieffer

principal ingredient – Cooper pairs (L.Cooper, 1956)

**attraction of two electrons** exchanging a virtual phonon

or **electron-phonon interaction**

**relation of spectral and superconducting characteristics**



$$k_B T_C = 1.14 \hbar \omega_D \cdot \exp \left( -\frac{1}{\lambda - \mu^*} \right)$$

$$\lambda = \frac{N_{el} \langle J^2 \rangle}{\langle M \omega^2 \rangle} = \frac{el - phon}{ion - ion}$$

SC-gap function

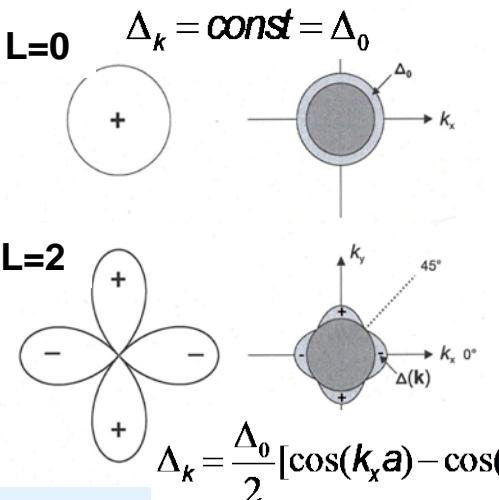
$$\Delta_k = - \sum_{k'} \frac{V_{kk'} \Delta_{k'}}{2 \sqrt{\epsilon_{k'}^2 + \Delta_{k'}^2}}$$

**retardation effect**  
**helps reducing the Coulomb repulsion**

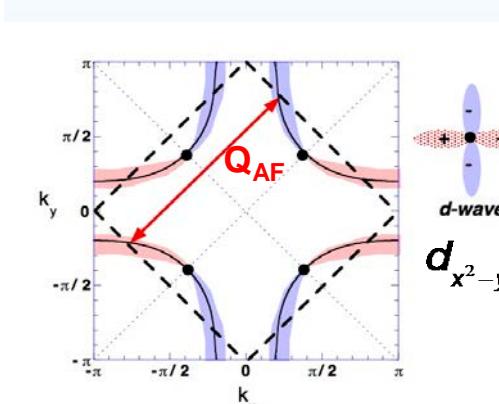
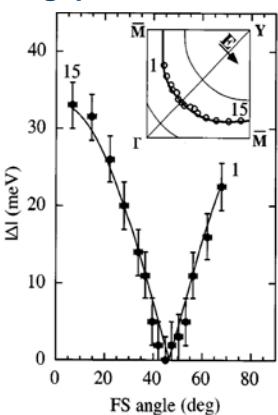
**electron pairs in BCS**  
**have zero spin and orbital momenta**  
**(the most symmetric state):**  
**L=0, S=0**

BCS:  
 $V < 0, \Delta = const > 0$

# «Unconventional» SC state in HTSC is experimentally proved



d-wave gap function: ARPES (1996)



For such gap symmetry

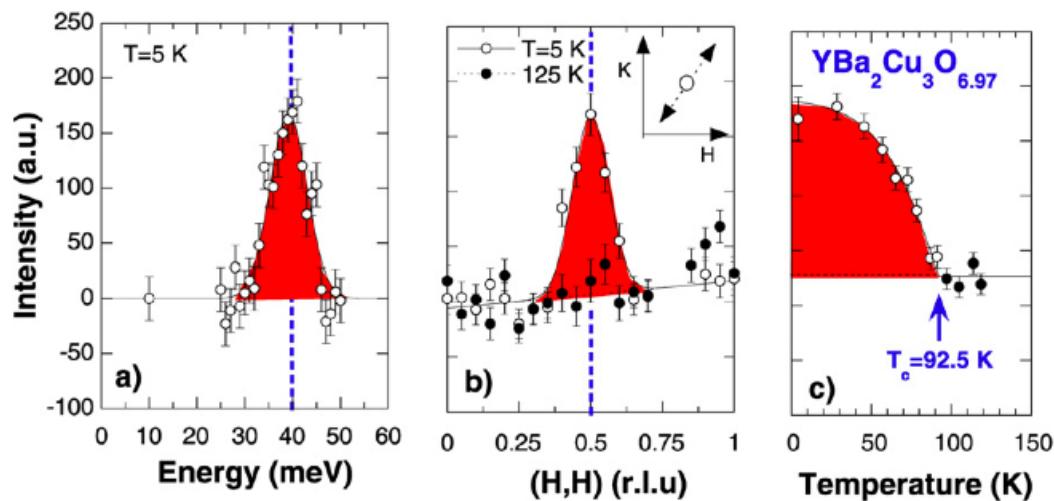
$$\chi''(Q, \omega)$$

in the SC state has increased value at certain  $Q$  (AFM-vector  $Q_{AF}$ ) in the plane

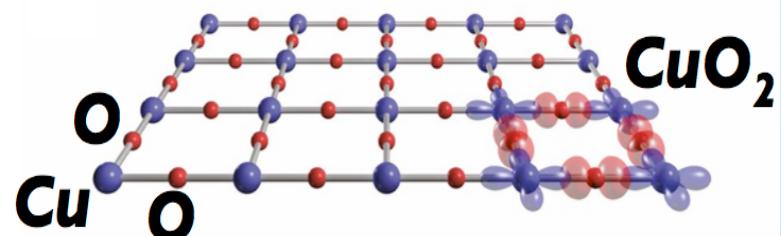
$L=2$   
d-wave pairing

$$\text{Intensity} \sim \chi_{\text{gap}}^{||}(Q, \omega) \sim \prod_k \left\{ 1 - \frac{\Delta_k \Delta_{k+Q} + \epsilon_k \epsilon_{k+Q}}{\sqrt{\Delta_k^2 + \epsilon_k^2} \sqrt{\Delta_{k+Q}^2 + \epsilon_{k+Q}^2}} \right\} F(k, Q, \omega)$$

The spin (or magnetic) resonance is observed by INS



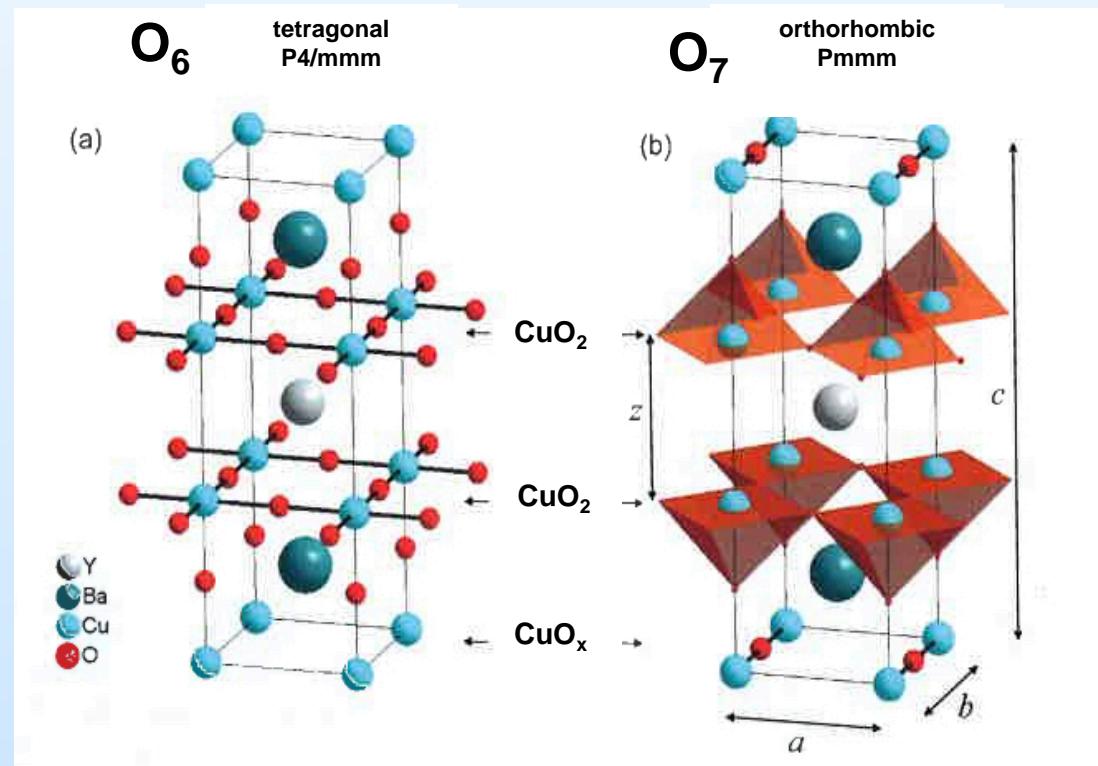
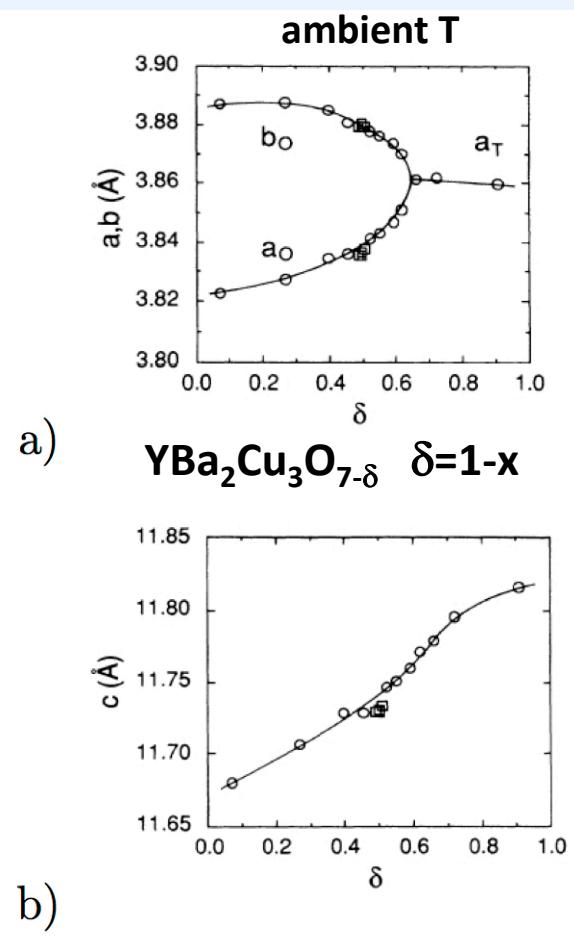
Common to all cuprates:  
the CuO<sub>2</sub> crystal layers



# Cuprates: complex oxides with a layered crystal structure

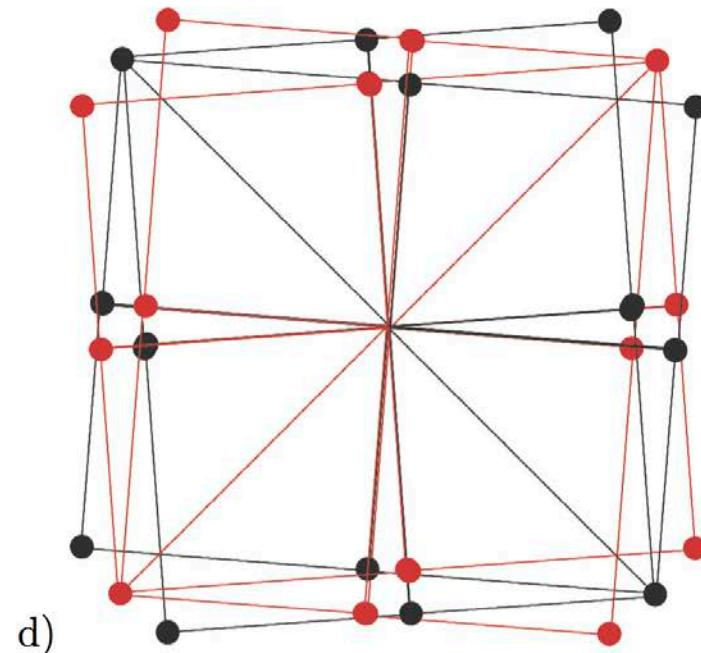
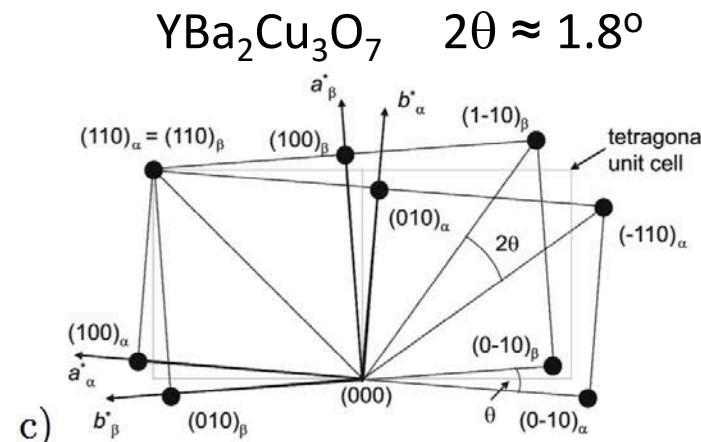
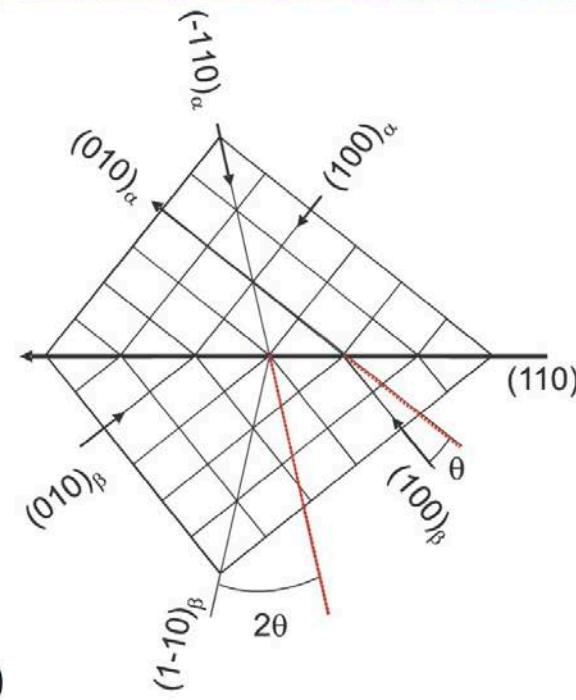
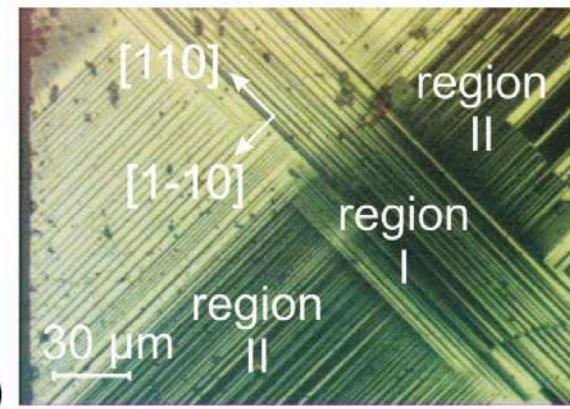
The layers  $\text{CuO}_2$  are responsible for the main SC properties while the other layers stabilize the crystal structure and serve charge “reservoirs”

## Perovskite-like layered structures



All are tetragonal at high temperatures (>500 K)  
tetra-ortho phase transition is doping dependent

# Orthorhombic structures: elastic domains



# Preparing single-domain (detwinned) samples

As grown crystals are first annealed in appropriate atmosphere in order to reach the desired doping content

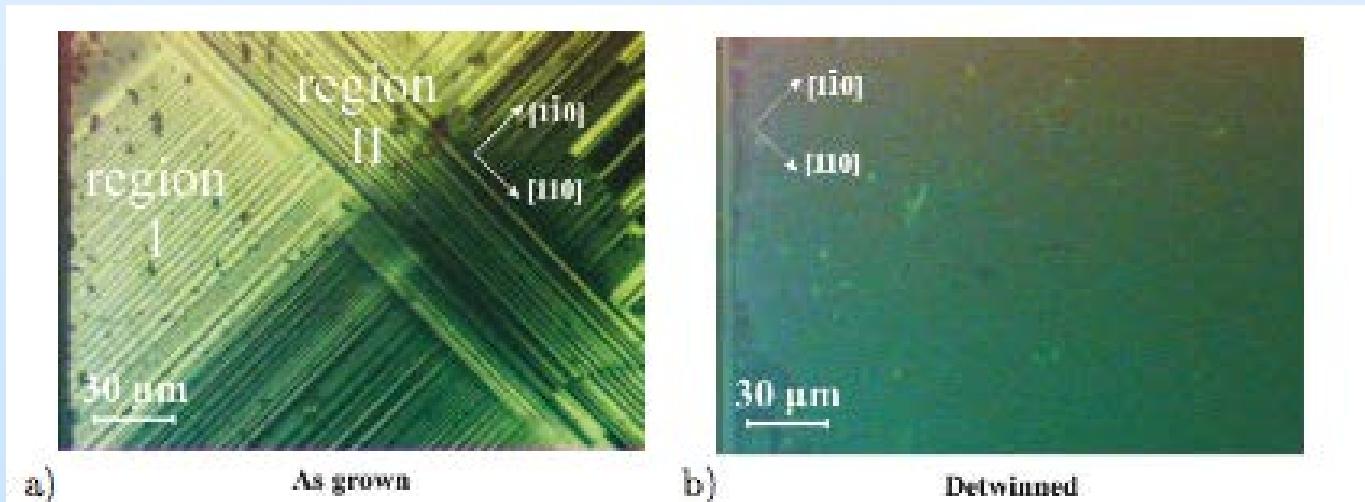
Then crystals, one after another are compressed with a uniaxial mechanical force (~0.5 kbar) applied along  $<100>$  ("a" or "b") at high temperature in the tetragonal phase while keeping a controlled atmosphere around the crystals

then cooled through the tetra-ortho transition keeping the force

and at last the force is released at ambient temperature

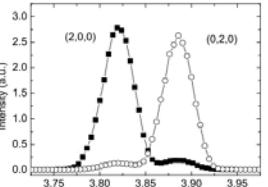
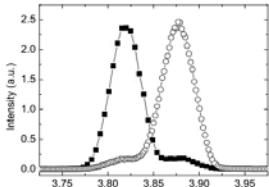
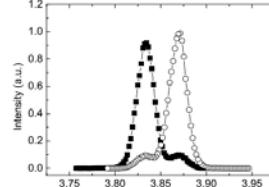
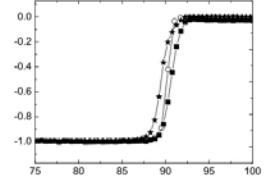
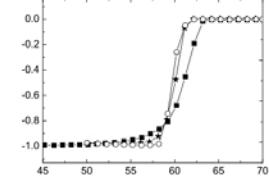
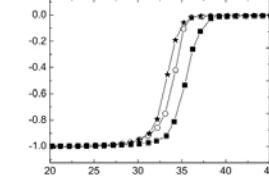
appropriate sample size – several cubic mm

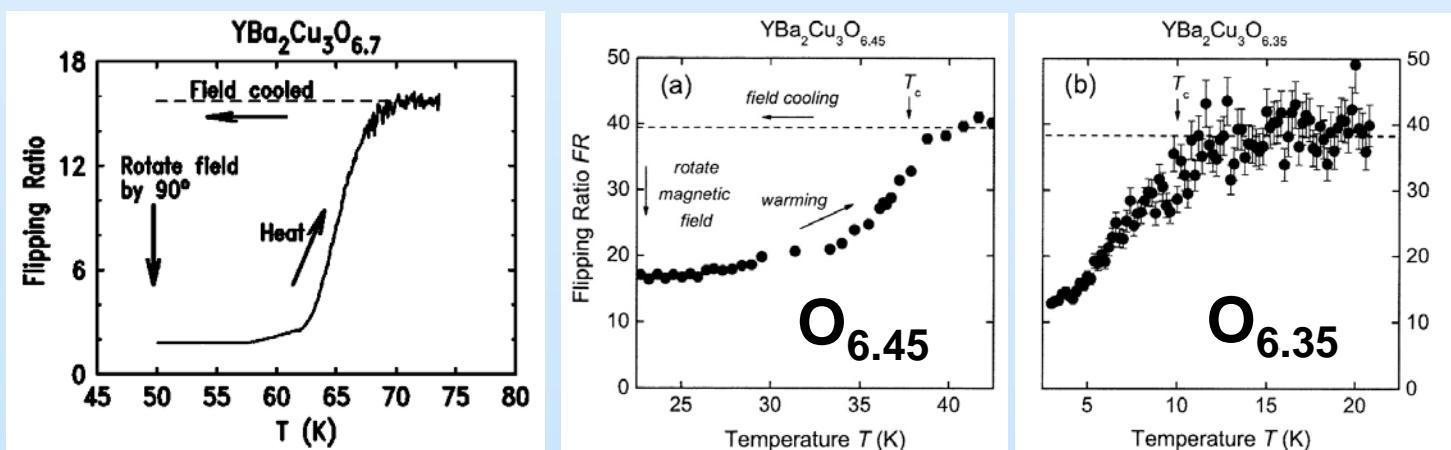
not enough for INS – composed samples from individually characterized crystals



# Preparing single-domain (detwinned) samples

## neutron beam characterization

Nominal composition	$\text{YBa}_2\text{Cu}_3\text{O}_{6.85}$	$\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$	$\text{YBa}_2\text{Cu}_3\text{O}_{6.45}$
$p_h$	0.148	0.12	0.085
mass (g)	1.3	2.9	2.0
majority domain	95%	94%	92%
elastic scans			
$T_{c,\text{mid}}(K)$ [ $\Delta T_c$ (K)]	90 [2]	61 [2]	35 [3]
typical curves			
$E_{\text{resonance}}$ (meV)	41	38	20 (?)



# Objects for research: single crystals

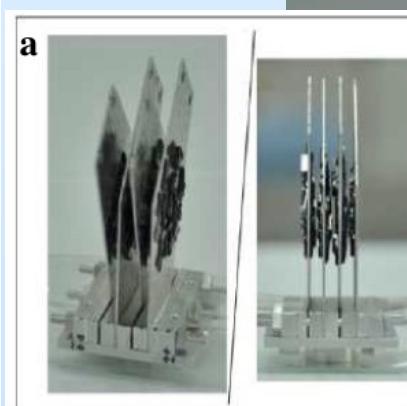
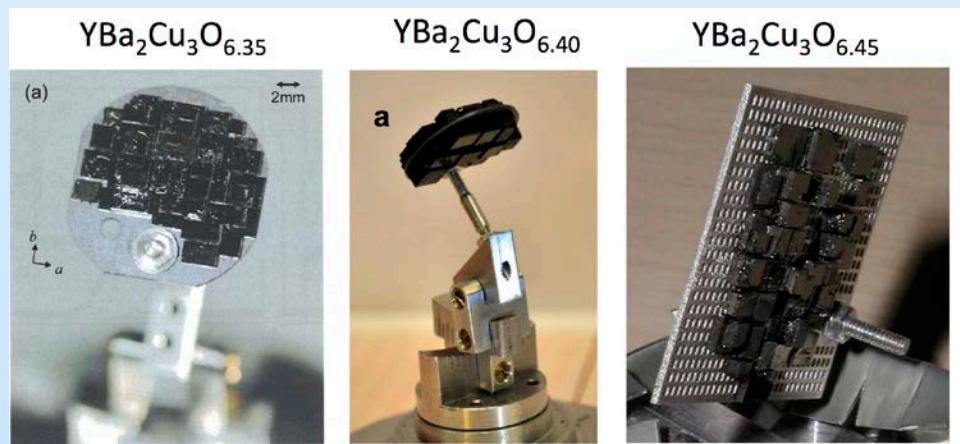
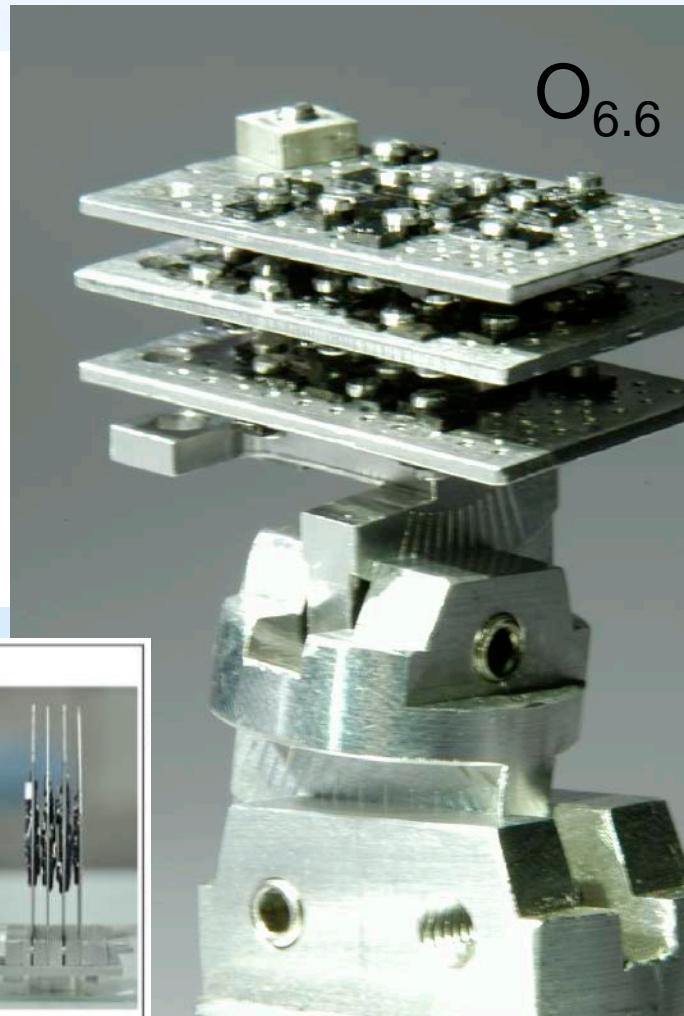
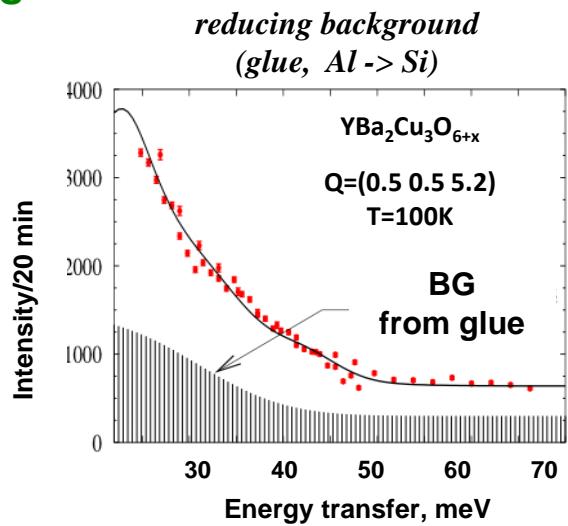
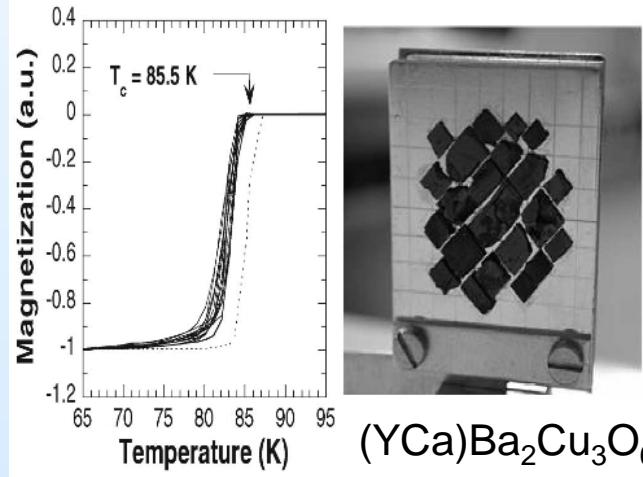
good to have  $\sim 1 \text{ cm}^3$

In the great majority of cases it is not possible  
in particular for new materials such as HTSC

«composed» samples:  $0.06\text{-}0.45 \text{ cm}^3$ ,

quality (mosaic spread) :  $1^\circ \text{ - } 2^\circ$

8, 60, 80, 120, 180, 250(!)  
small single crystals



# Experimental equipment

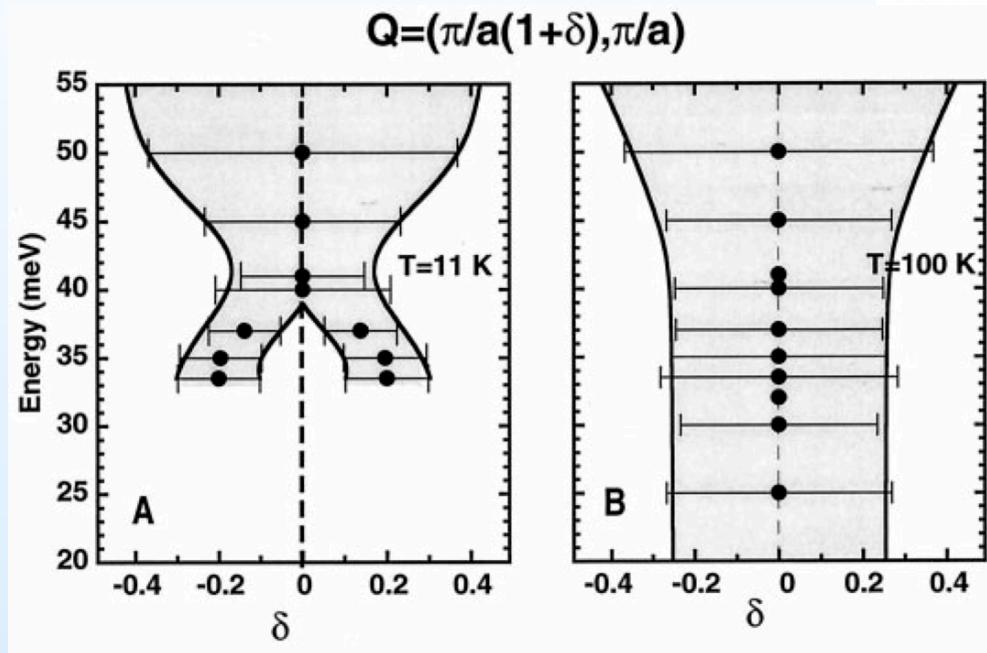
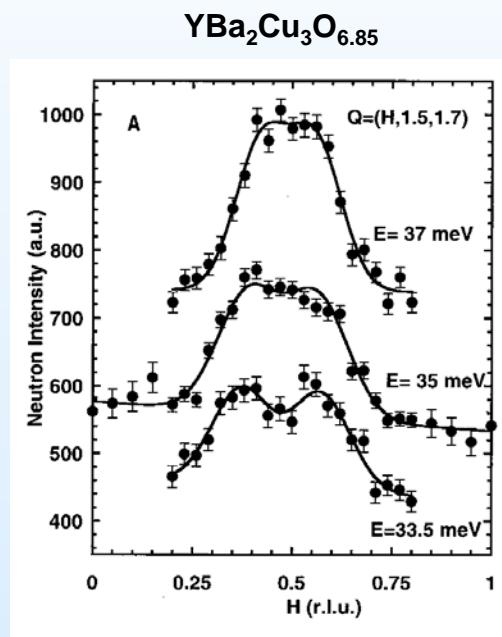


**“On the-floor”**  
distances – meters  
divergences - degrees

weight of the moving modules – up to tons  
precision of positioning – 0.01 degree

neutron polarization analysis

# Dispersion of the resonance intensity



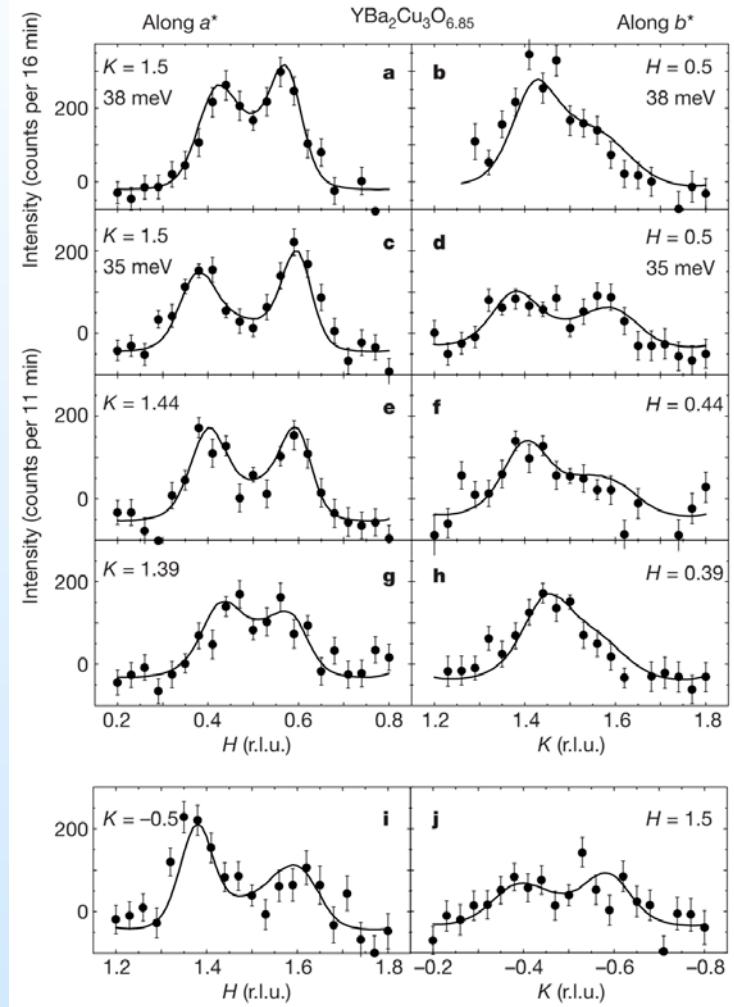
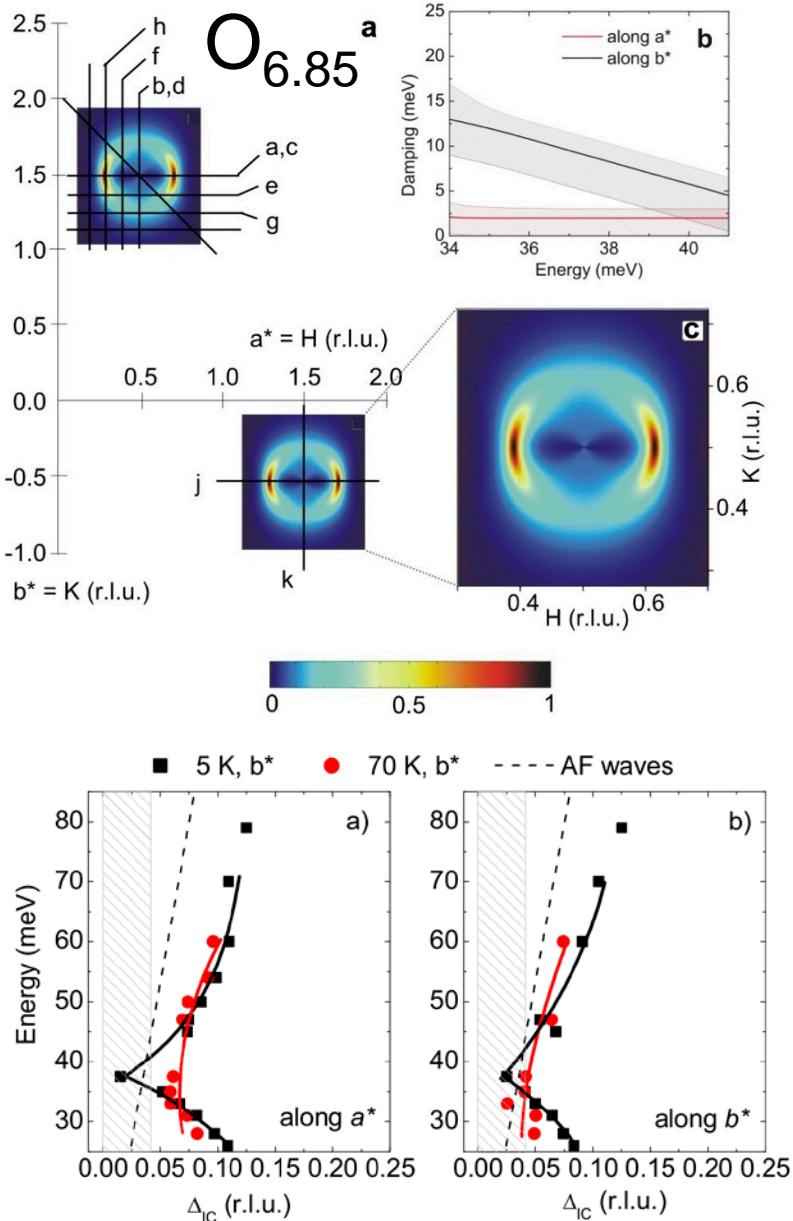
incommensurability of the signal below  $T_c$

cannot be related to pinned “stripes”

more detailed analysis on detwinned samples

# Magnetic resonance in cuprates

anisotropy in the plane  $\text{CuO}_2$  and dispersion of the resonance intensity

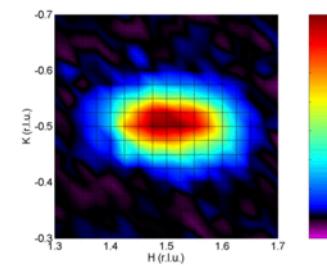
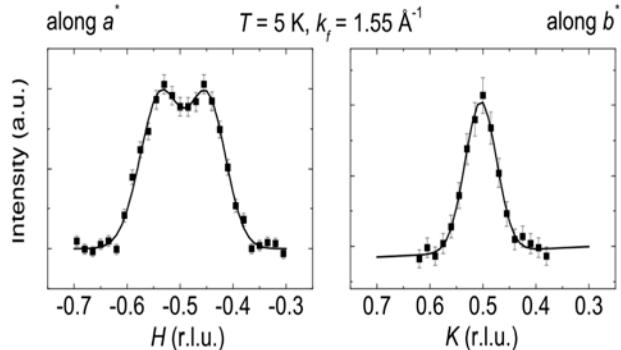
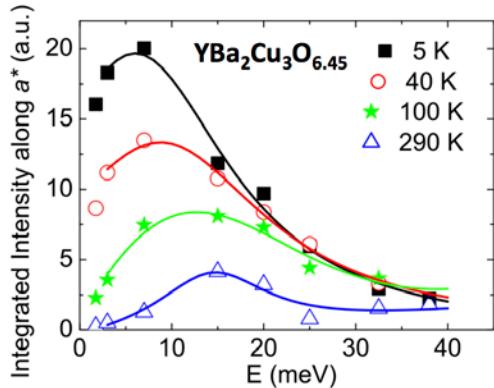


Anisotropy of the forms "X" and "Y"  
(below and above T<sub>c</sub>)

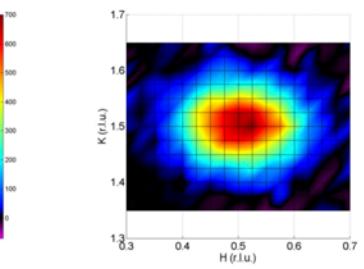
nematic electron correlations: 2D

# Magnetic resonance in cuprates

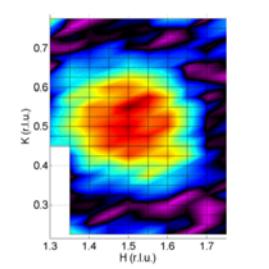
## anisotropy in the plane $\text{CuO}_2$ and the resonance dispersion



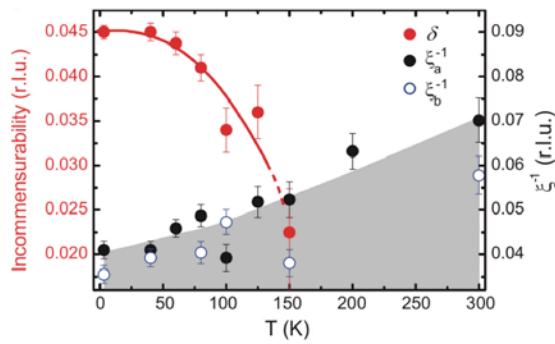
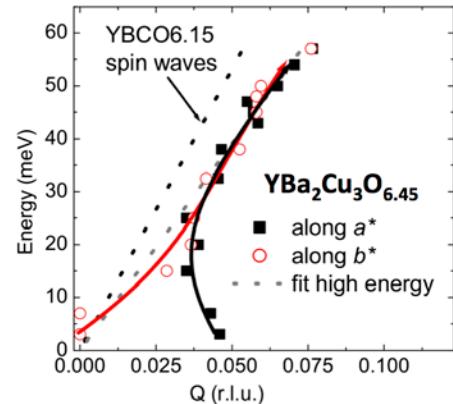
a) 3 meV,  $k_f = 2.66 \text{ \AA}^{-1}$



b) 7 meV,  $k_f = 2.66 \text{ \AA}^{-1}$



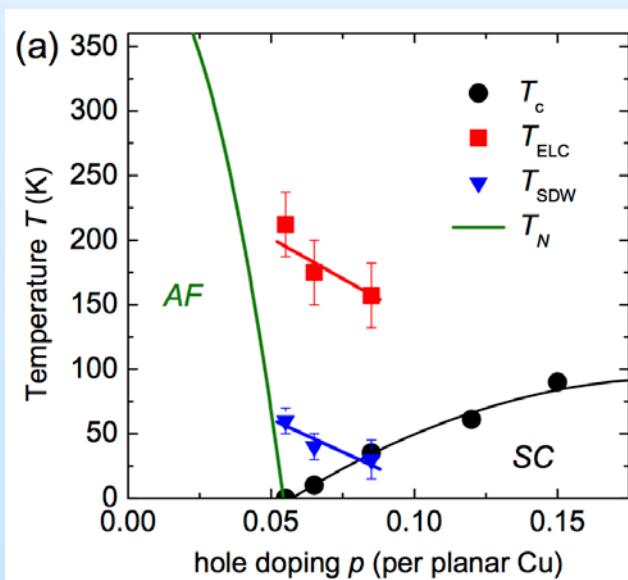
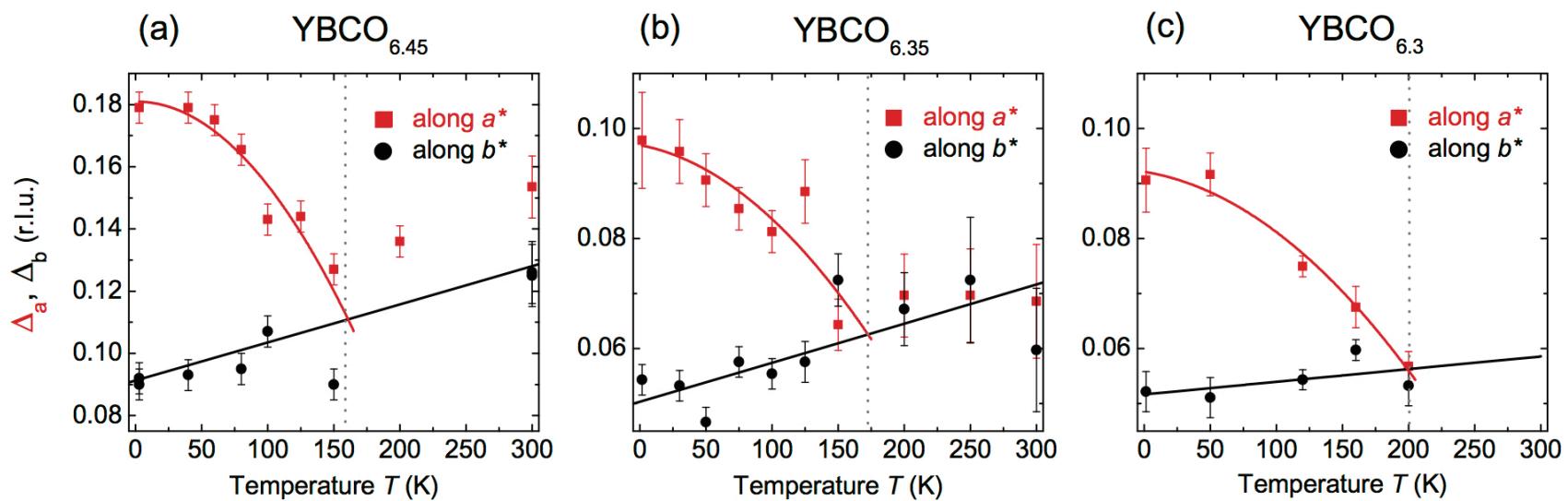
50 meV,  $k_f = 4.1 \text{ \AA}^{-1}$



anisotropy in the plane increases at lower energies  
and  
with reducing doping “x” in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

# Magnetic resonance in cuprates

## anisotropy in the plane $\text{CuO}_2$ and the resonance dispersion



# Fe-based SC

(from 2008 – pnictides, then selenides)

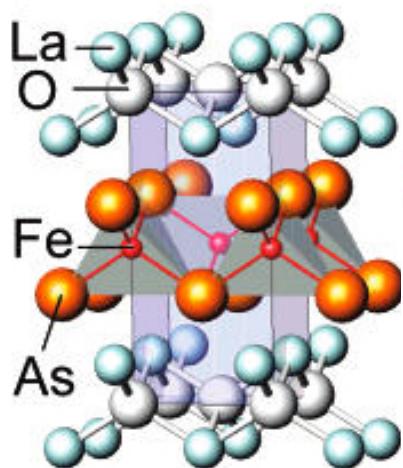
resemble cuprates: layered structures, Magnetic AFM layers, several structure types, phase diagrams alike



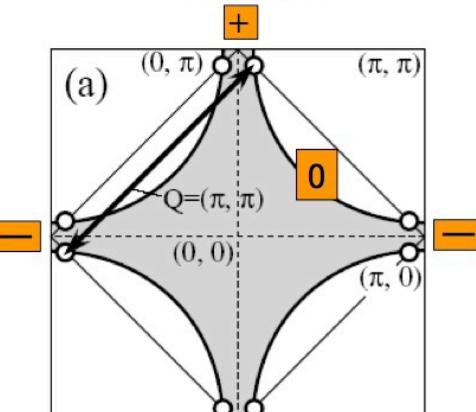
LaOFeAs

Kamihara et al

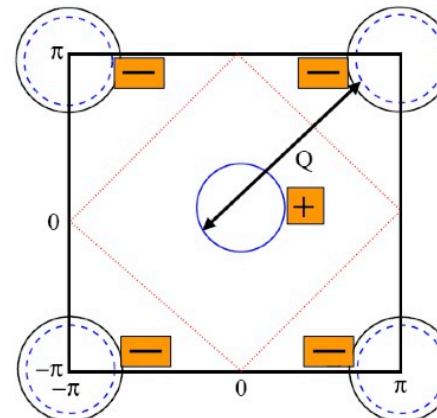
IACS 2008



## Cuprates



## Pnictides

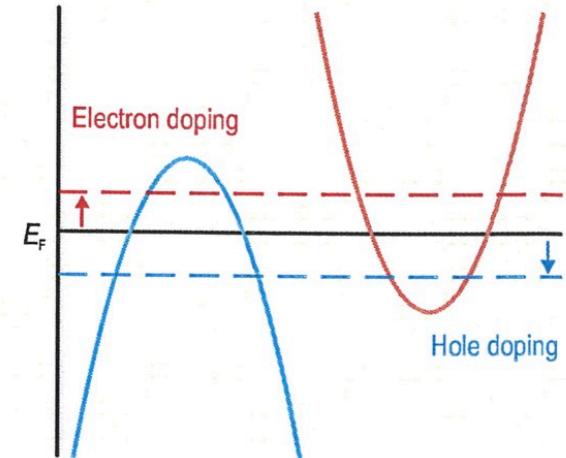
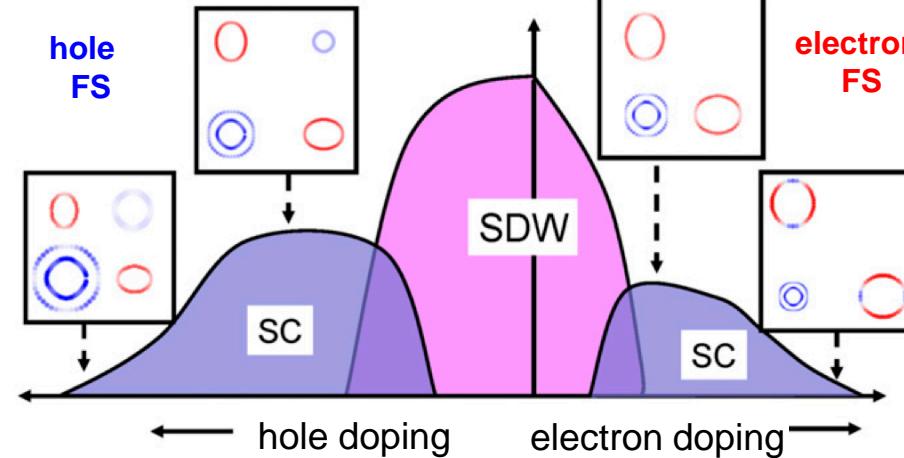
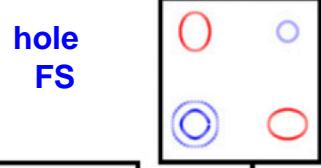


Resonance:

interband transitions between distinct parts of the Fermi surface with different signs of the SC-gap function:

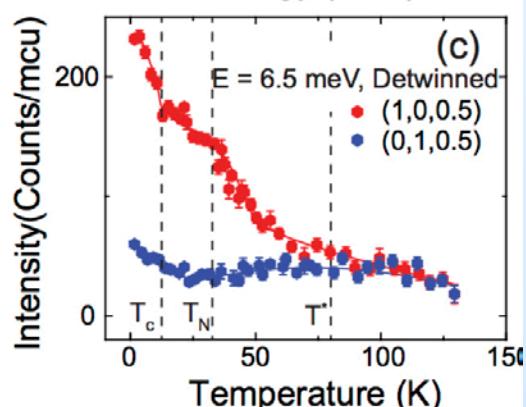
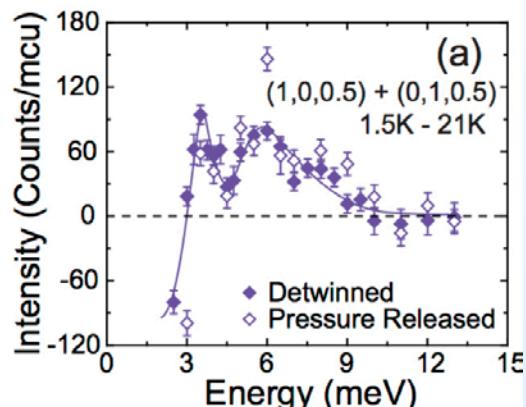
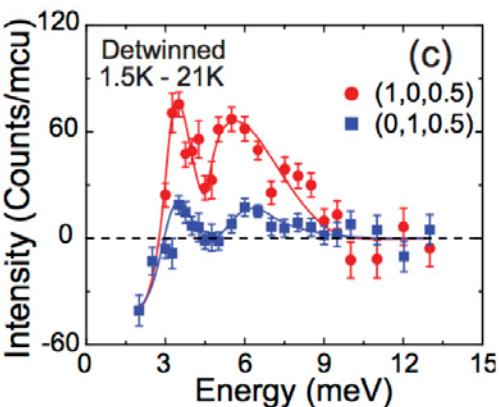
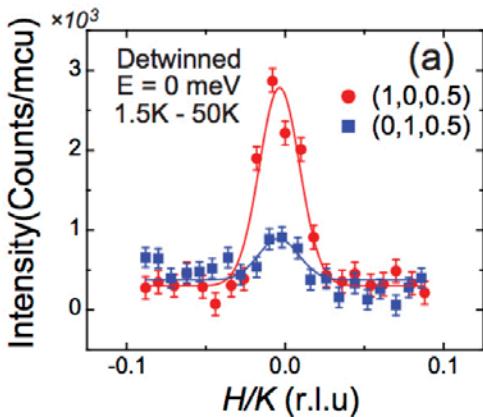
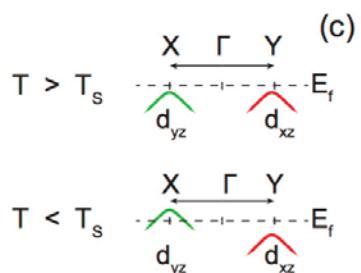
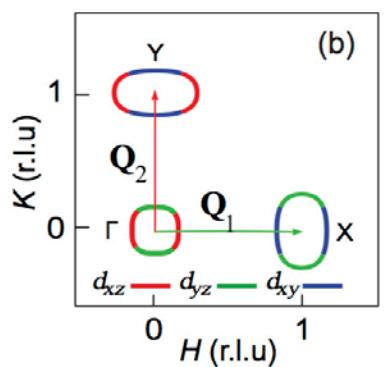
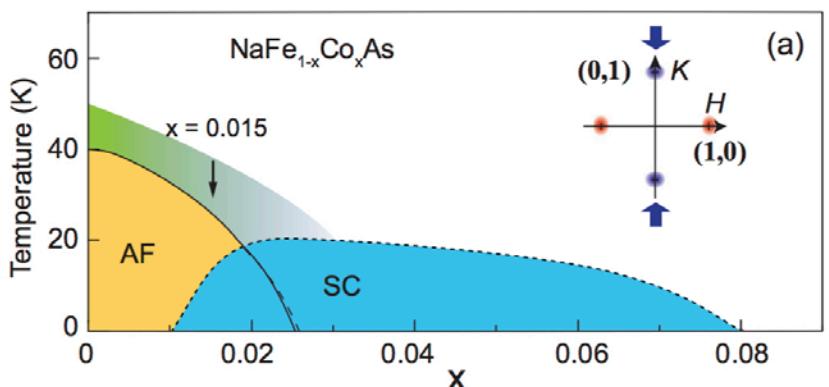
$$\Delta(\mathbf{k}) = -\Delta(\mathbf{k}+\mathbf{Q}_{AF})$$

so called  $S^{\pm}$  pairing

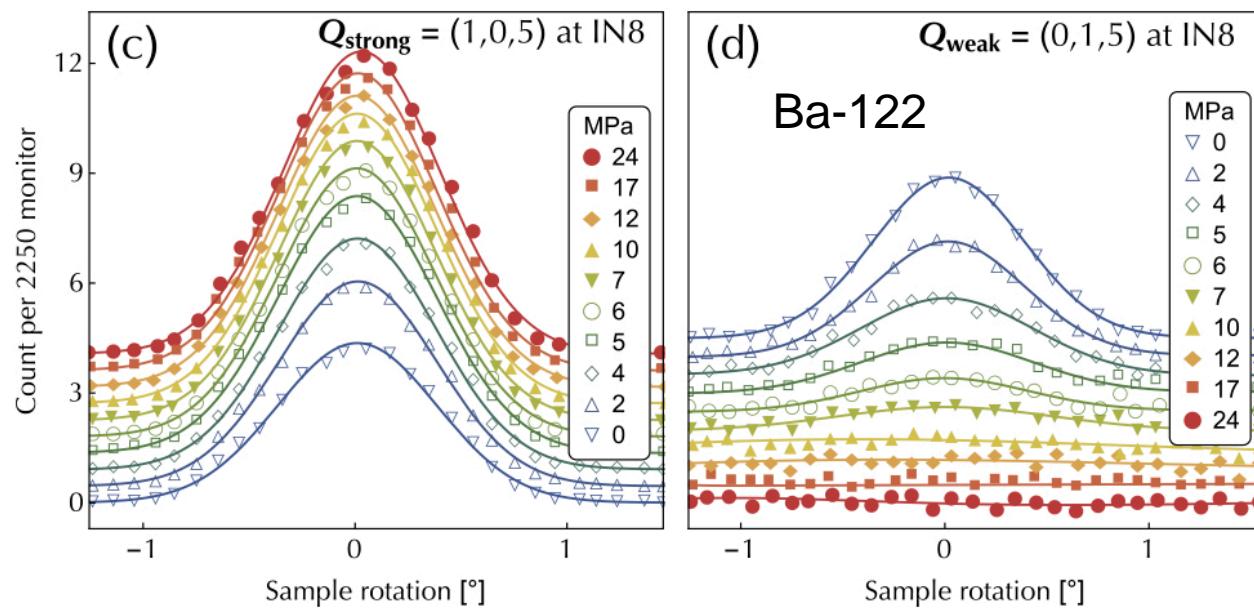
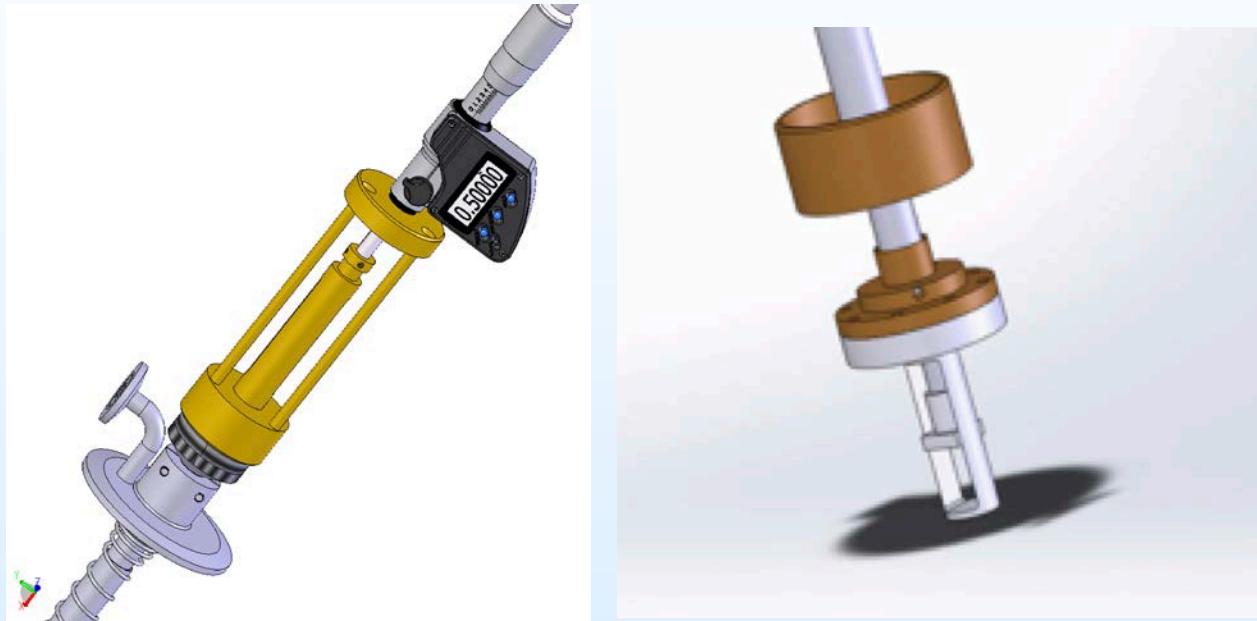


# Anisotropy of the magnetic resonance in the 111 family Na(FeCo)As

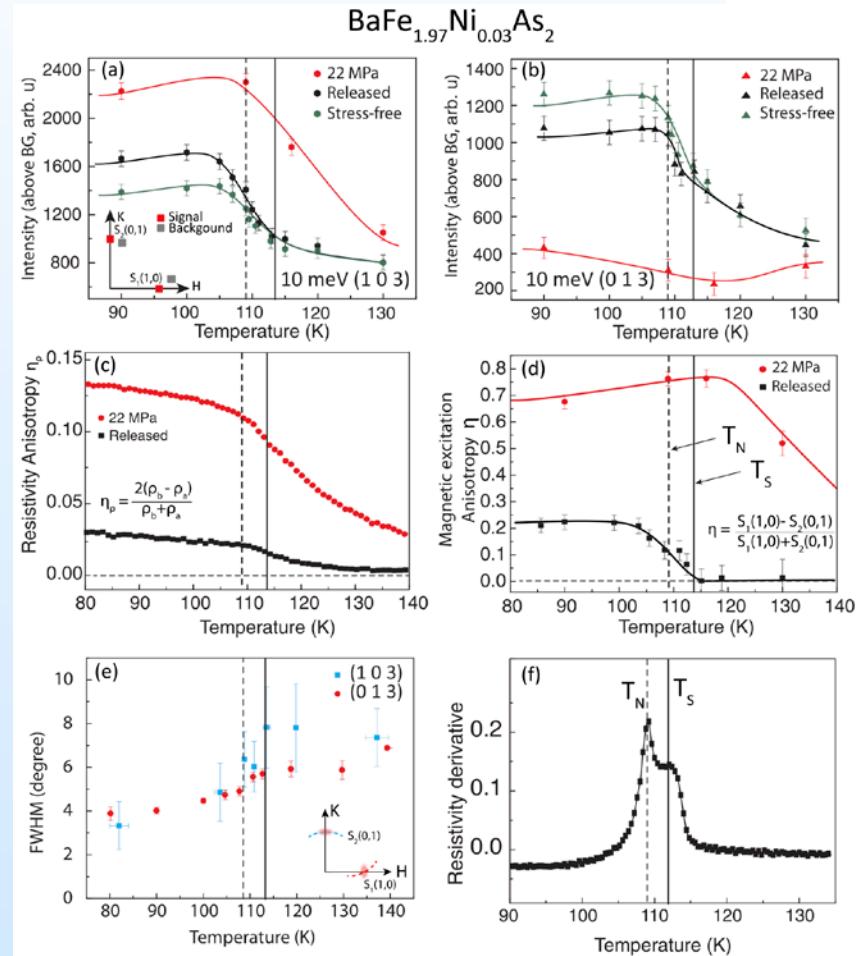
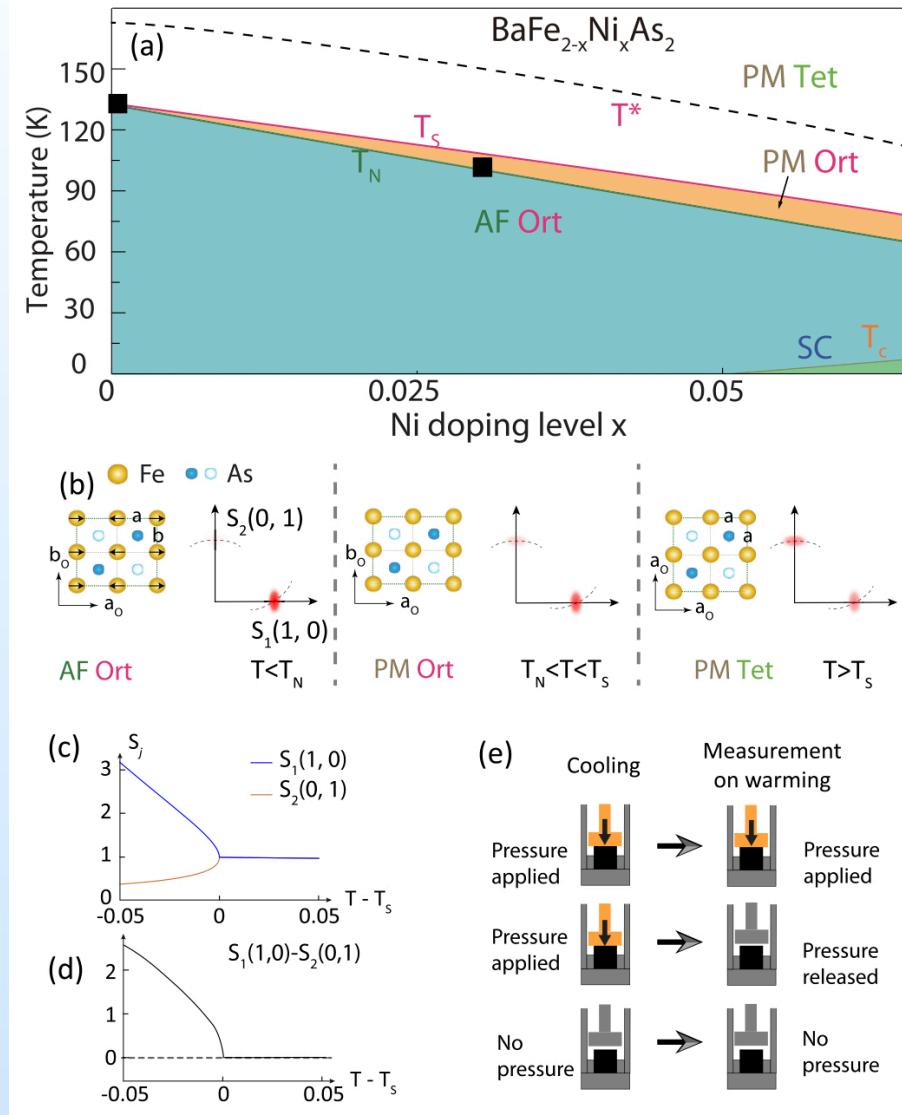
lifting of the orbital degeneration under uniaxial stress



# *“In-situ”* detwinning under uniaxial stress at low temperature



# “*In-situ*” detwinned Ba-122



Anisotropy begins at structural transition ( $T_s$ )

# Conclusion



**Anisotropy of magnetic fluctuations is well developed  
in the orthorhombic phases of  
copper- and iron-based unconventional superconductors**

**Anisotropy of magnetic fluctuations  
is supportive of the theories  
generating nematic order in the 2D electronic liquid**

**the “broken symmetry” low-temperature phases  
correspond to reduced rotational  
and not  
translational symmetry**



# ВТСП на основе железа

(с 2008 года – пникиды, и затем - селениды)

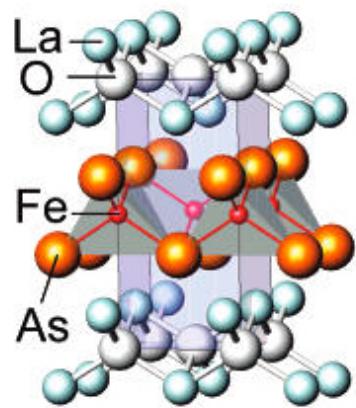
во многом похожи на купраты:

структуры со слоями, есть магнитно-активные слои с AFM взаимодействием  
несколько типов структур, подобные фазовые диаграммы

LaOFeAs

Kamihara et al

JACS 2008



Слоистые структуры, но с тетраэдрической, не планарной координацией

Другие различия: недопированные соединения – не изоляторы, а металлы, хотя и «плохие»

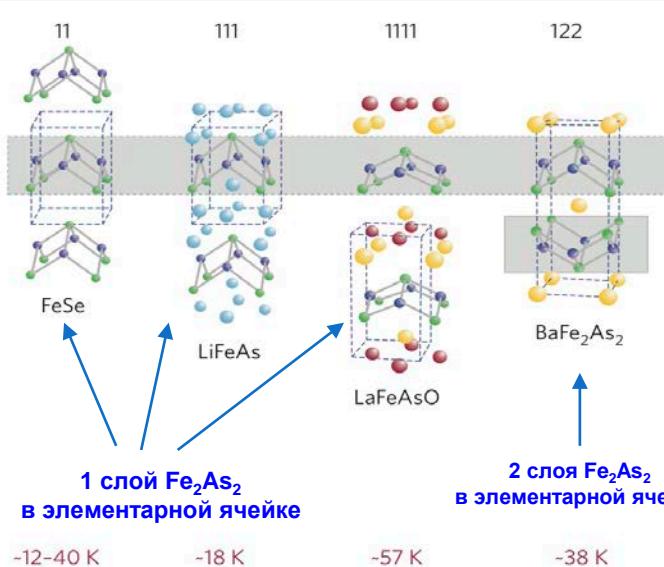
Допирование в Fe-based: все типы возможны, электронные, дырочные, изовалентные, за счет изменения расстояний под давлением.

Можно широко замещать Fe, тогда как в купратах СП быстро деградирует при замещении Cu (1%).

Купраты более однородны внутри семейства, а Fe-based могут сильно отличаться по свойствам

Fe based более сложные:

много-зонные, много-орбитальные,  
много-щелевые



-12-40 K

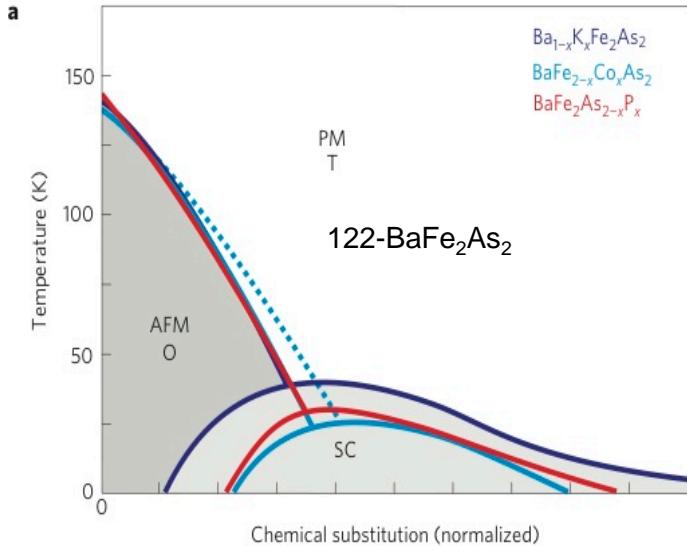
-18 K

-57 K

-38 K

Paglione et al, Nat.Phys. 2010

a



122-BaFe<sub>2</sub>As<sub>2</sub>

Вдвое более плотное «заселение»  
магнитных ионов Fe в слоях:  
Fe<sub>2</sub>As<sub>2</sub> против CuO<sub>2</sub>  
с примерно одинаковым  
размером ячейки

Metal iron (bcc):

$a = 2.866 \text{ \AA}$

$\text{Fe-Fe} = 2.480 \text{ \AA}$

Magnetic moment

$\text{Fe} = 2.2 \mu_B$

Fe<sub>2</sub>As<sub>2</sub>: Fe-Fe = 2.70 -

2.80 \AA

● Fe ( $z = 0$ )

● As ( $z \neq 0$ )

Spin Fe<sup>2+</sup> ( $d^6$ ):

$S=2$

Magnetic moment Fe

$0.1 - 3.4 \mu_B$

CuO<sub>2</sub>: Cu-Cu = 3.85 - 4.0

● Cu ( $z = 0$ )

● O ( $z = 0$ )

● Spin Cu:

$S=1/2$

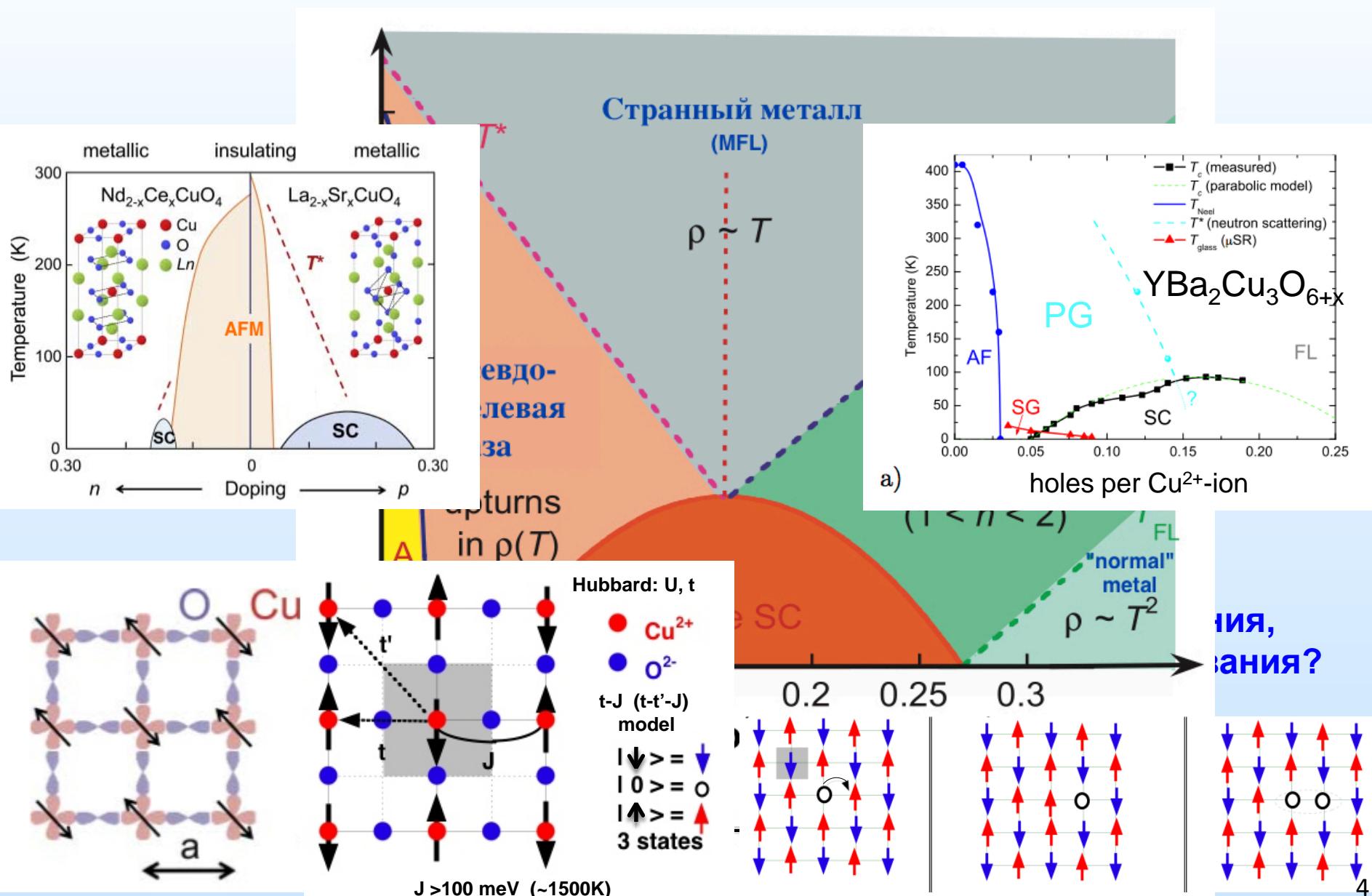
Magnetic moment Cu

$\sim 0.5 \mu_B$

Широкая вариация  $T_N$  и моментов

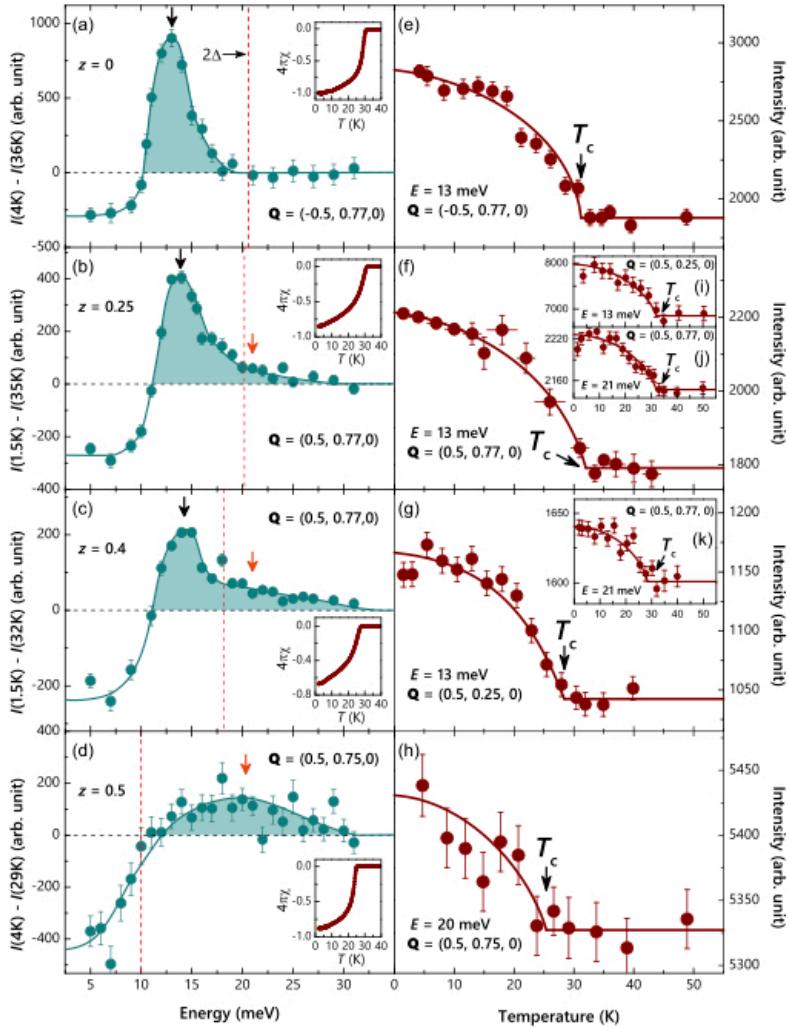
# Фазовые диаграммы

Общее: СП возникает при зарядовом допировании  
(электронном или дырочном) плоскостей CuO<sub>2</sub>

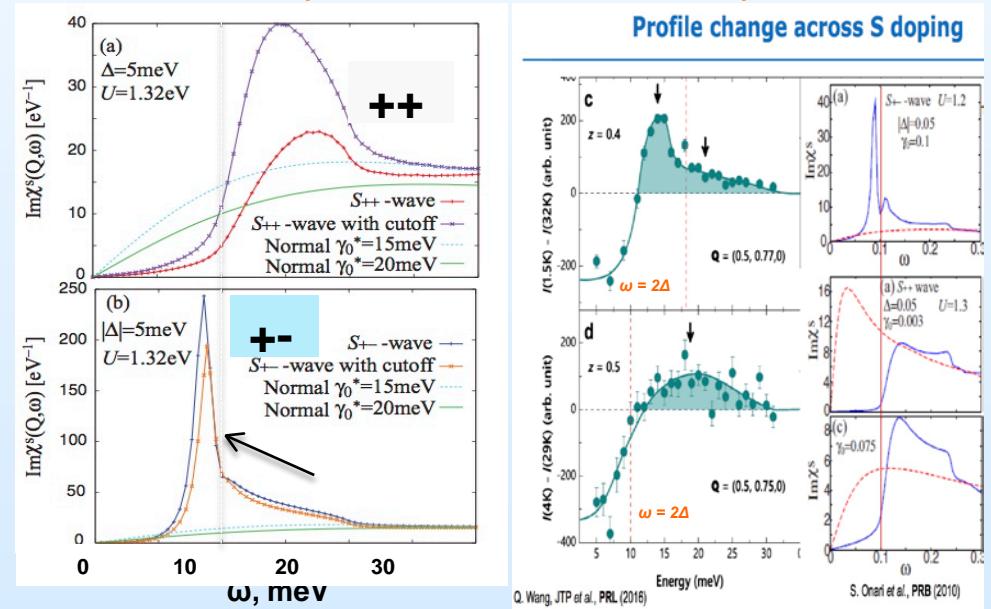


# Полученные данные: пример магнитное рассеяние в S-замещенных селенидах

Изменение типа спаривания в одном семействе  $K_xFe_2(Se_{1-z}S_z)$   
при легировании серой – малые изменения  $T_c$ , подобные свойства

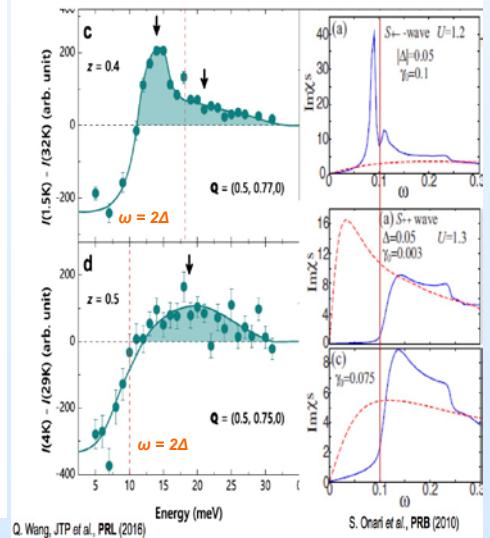


Наблюдаемые изменения похожи на то, что было  
рассчитано для  $S^{++}$  и  $S^{+-}$  магнитных откликов  
(S.Onari et al PRB 2010, 2011)



Q. Wang, JTP et al., PRL (2016)

Profile change across S doping



S. Onari et al., PRB (2010)

По мере увеличения содержания серы магнитный  
резонанс возникающий, по имеющимся представлениям,  
в симметрии  $S^{+-}$ , прогрессивно исчезает и замещается  
«нерезонансным» поведением, характерным для  
симметрии  $S^{++}$ .

Мы интерпретируем это как плавный переход  
от одного типа спаривания к другому.

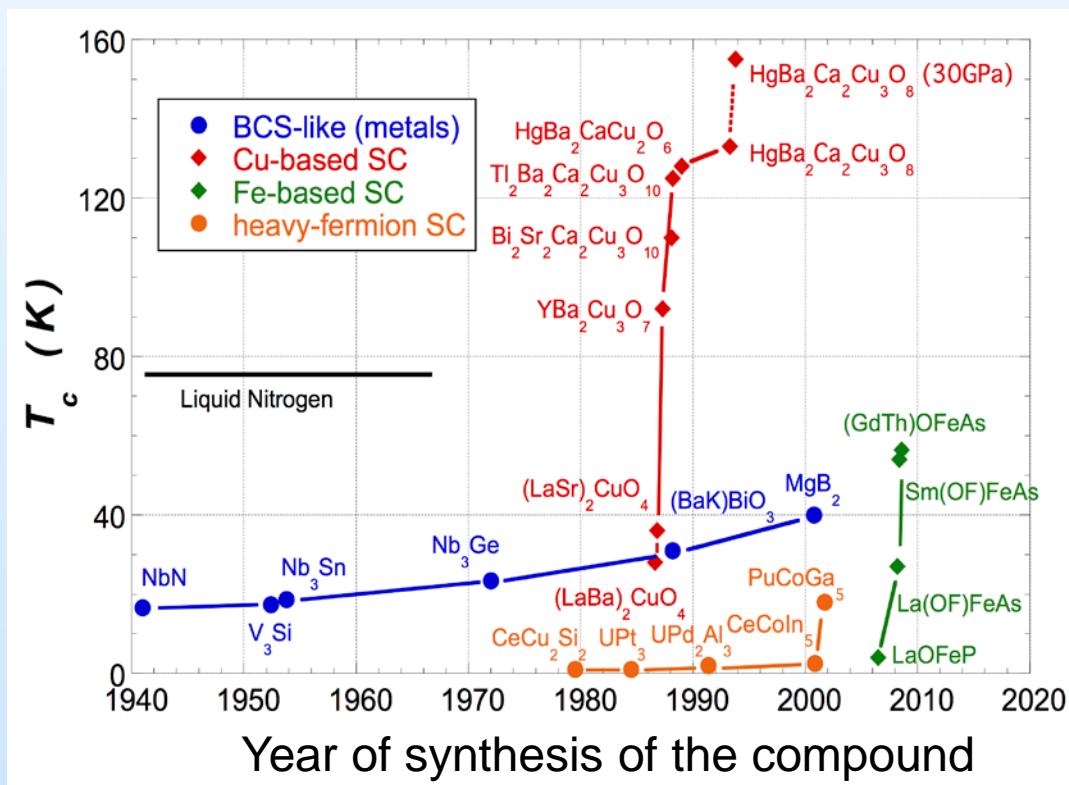
# High-Temperature Superconductors (HTSC) from 1986: $T_c > 30$ K

HTSC Cu-based:

oxides

HTSC Fe-based:

pniictides and chalcogenides



«Unconventional»  
superconductors  
ceramics materials

different from

«conventional», «usual»  
superconductors  
known earlier in metals  
and intermetallics

new mechanism of superconductivity