MMM, UCSB

Intermediate Order in the Cuprates

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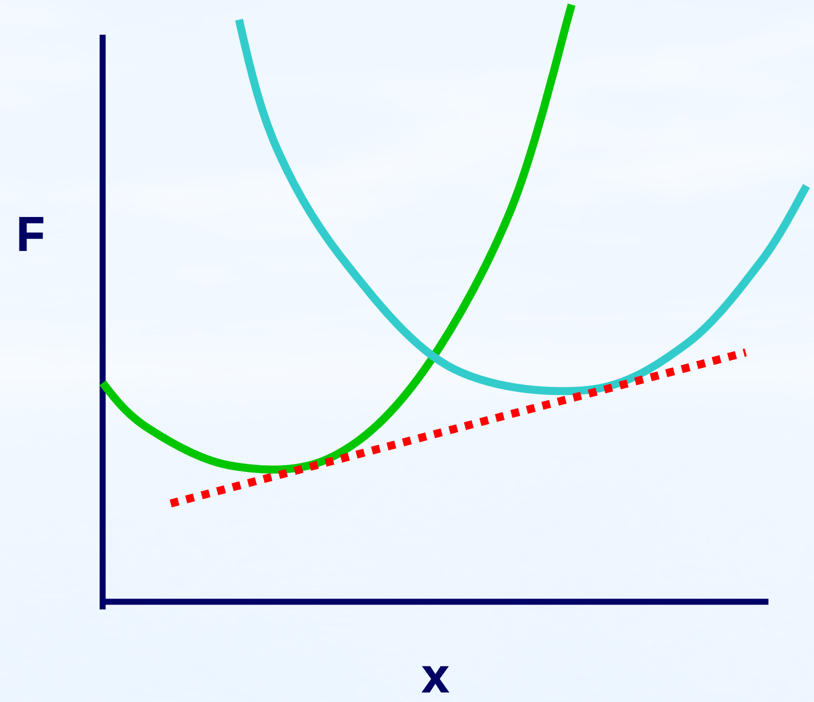
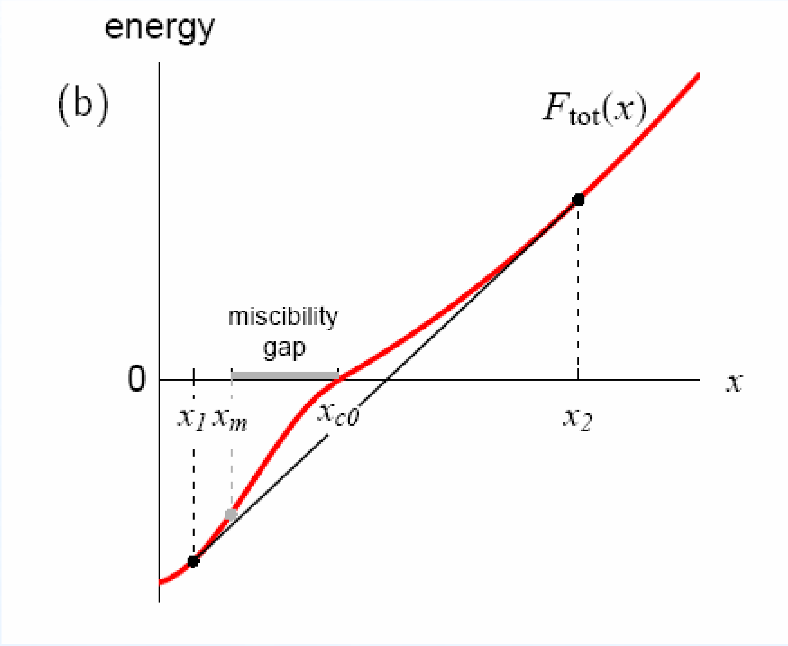
Outline

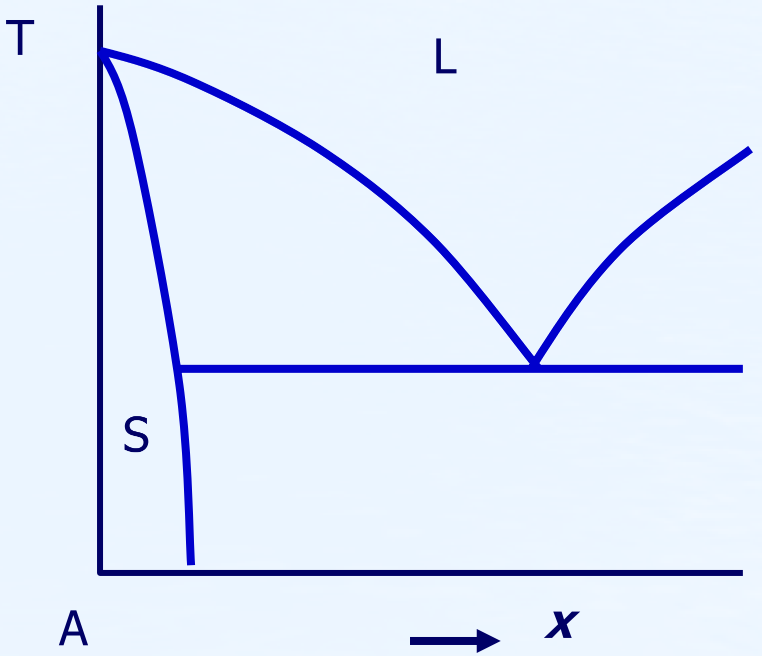
- **Nano-scale electronic phase separation in the manganites and the cuprates.**
- **Nature of the pseudo-gap state in the cuprates.**
- **Recent data with neutron scattering and Dark Matter in the cuprate physics.**
- **The possibility of intermediate order and a scenario of the spin-lattice synergy in the HTSC.**

Phase Transition and Phase Separation

- Phase transition is a recipe for phase separation; water and ice.
- Similar argument for the second order transition.



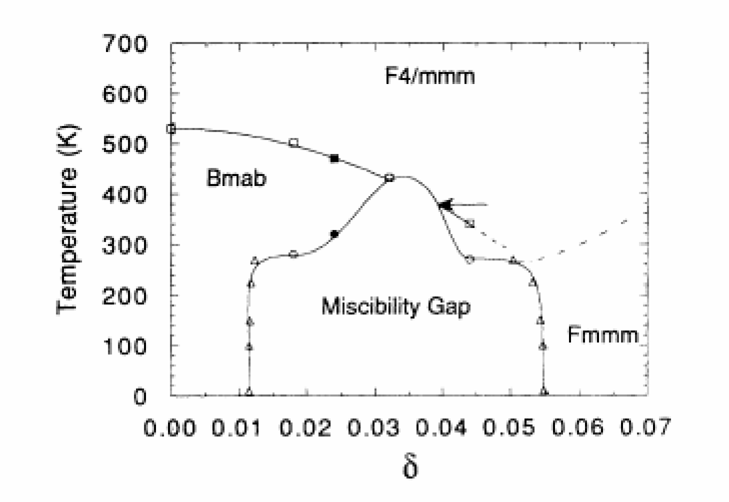




Electronic Phase Separation

- Macroscopic phase separation occurs if atoms are mobile.
- If electronic mobility is high but atomic mobility is absent, **phase separation with charge** occurs (V. Emery and S. Kivelson, E. Dagotto, et al.).
- Long-range Coulomb attraction and short range repulsion for phase separation creates the medium-range order (A. R. Bishop).

$La_2CuO_{4+\delta}$



P. G. Radaelli, et al., *Phys. Rev. B* **49,** 6239 (1994).

Physica C 209 (1993) 597–621
North-Holland

PHYSICA C

Frustrated electronic phase separation and high-temperature superconductors

V.J. Emery
Dept. of Physics, Brookhaven National Laboratory, Upton, NY 11973, USA

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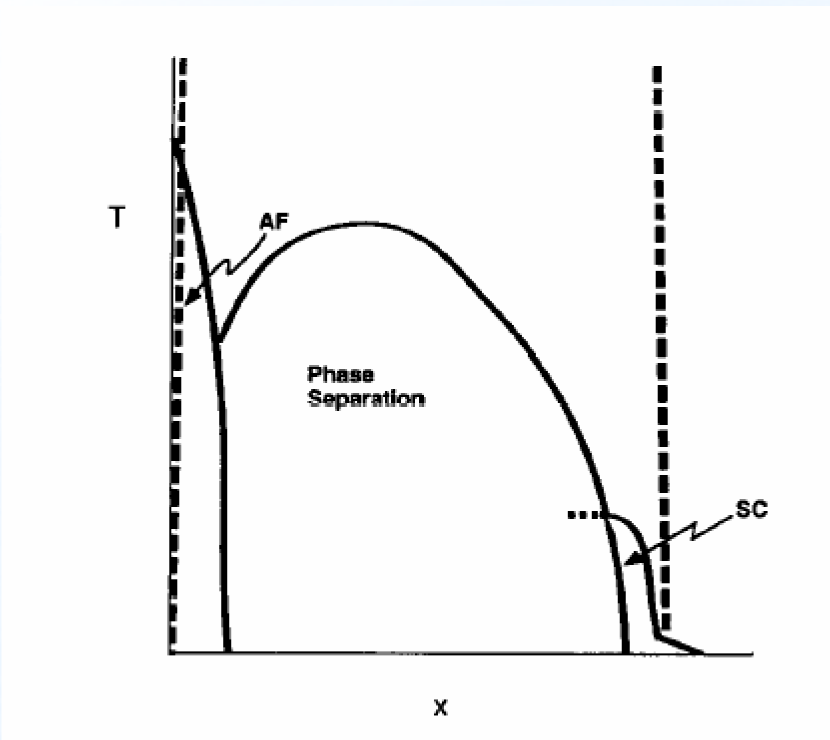
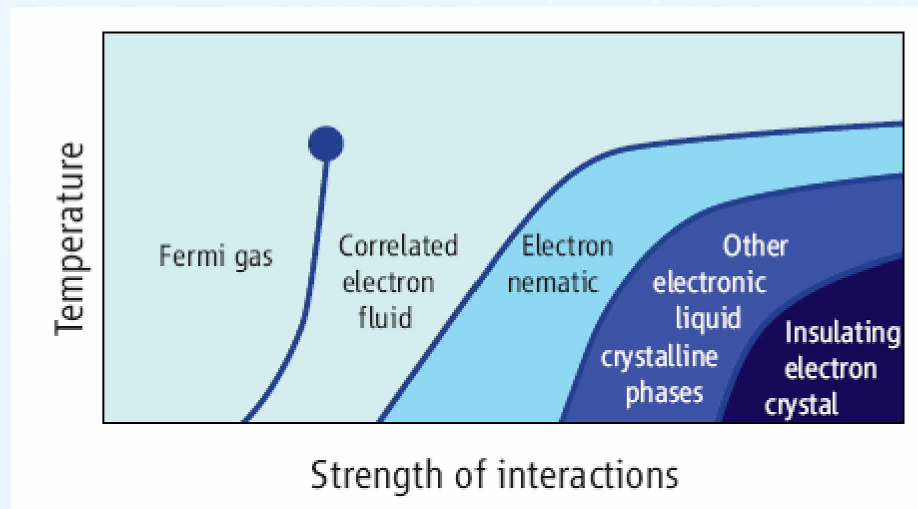
Dept. of Physics, UCLA, Los Angeles, CA 90024, USA

Received 22 December 1992

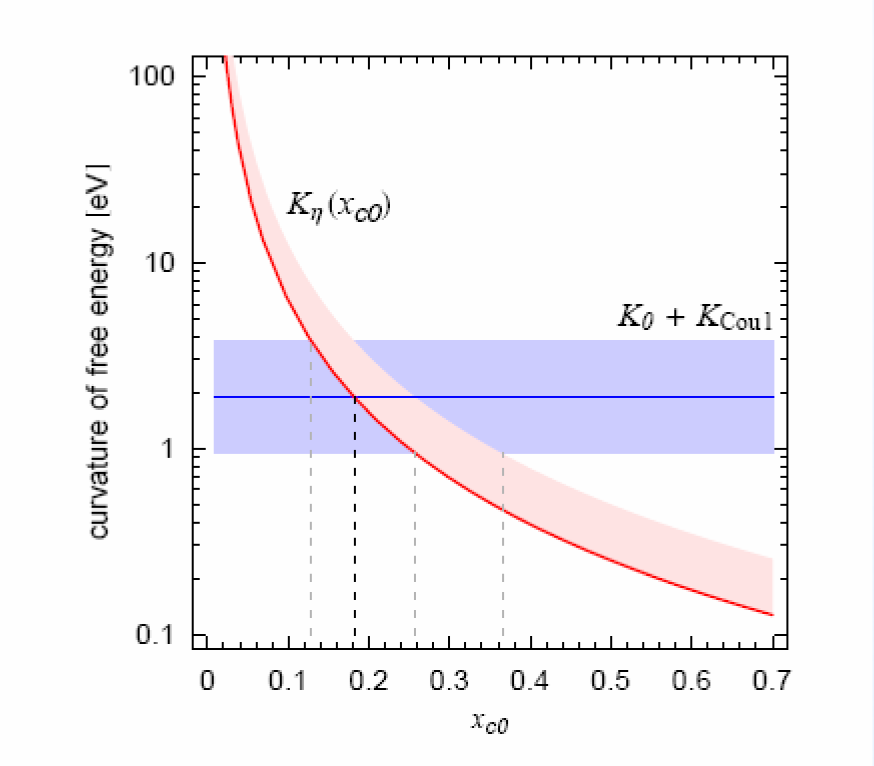




E. Fradkin, S. A. Kivelson and V. Oganesyan, *Science* **315**, 196 (2007)

Electronic Phase Separation in the Cuprates

- Realistic model calculation.
- Phase separation for 0.12 < x < 0.26.
- Self-organization into nano-scale phases, including the "lasagna" model (pasta model in cosmology).



B. Fine and T. Egami, cond-mat/0707.3994

Nano-Phase Separation in Manganites

Journal of Solid State Chemistry **151**, 323–325 (2000)
doi:10.1006/jssc.2000.8703, available online at http://www.idealibrary.com on IDEAL®

RAPID COMMUNICATION

High Dielectric Constant in $ACu_3Ti_4O_{12}$ and $ACu_3Ti_3FeO_{12}$ Phases

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Received February 29, 2000; accepted March 3, 2000

PHYSICAL REVIEW B **75**, 115129 (2007)

Giant dielectric permittivity and magnetocapacitance in $La_{0.875}Sr_{0.125}MnO_3$ single crystals

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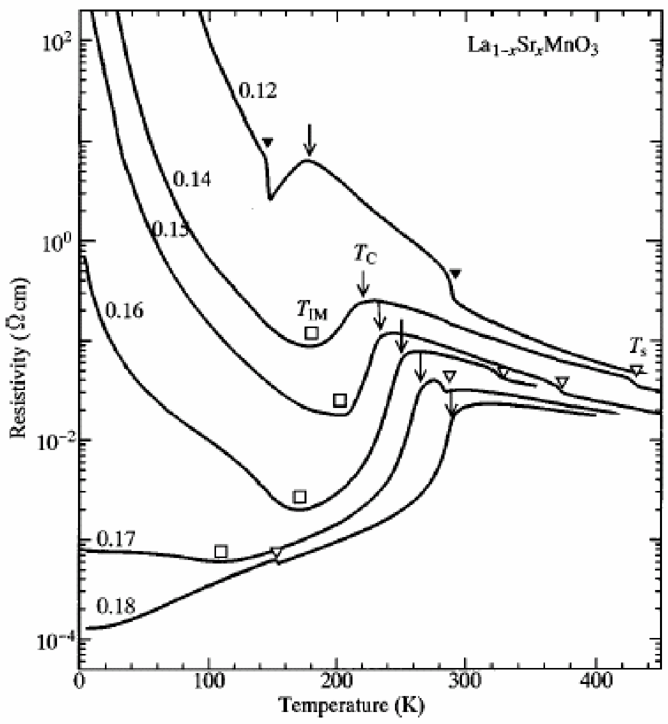
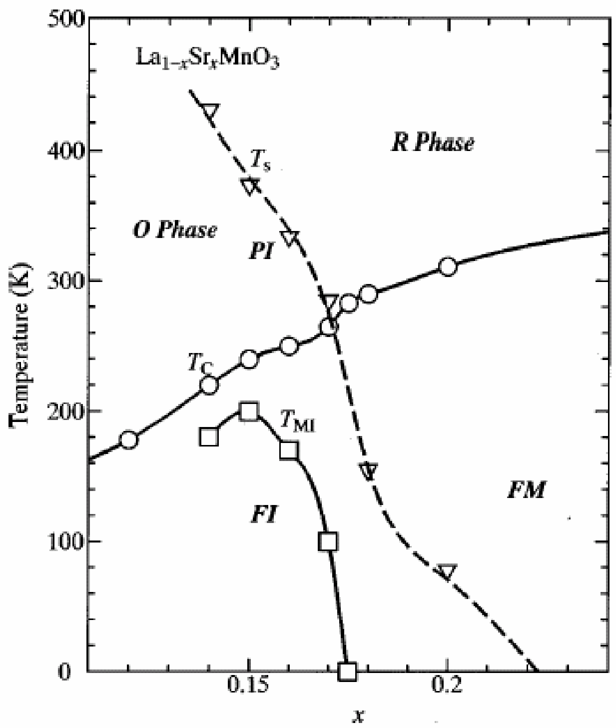
(Received 6 December 2006; published 29 March 2007)

Phase Complexity in LSMO



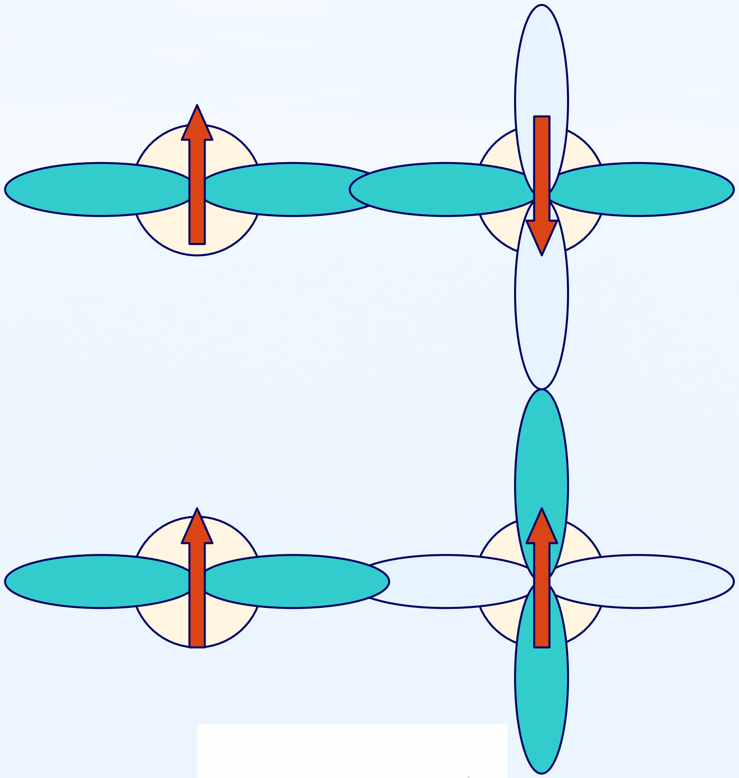


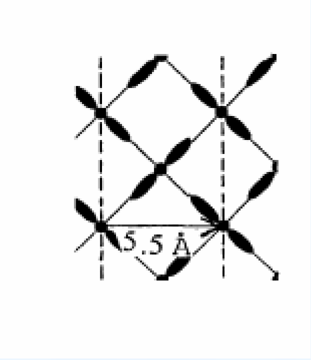
A. Moritomo, et al, PRB 56, 12190 (1997)

- $La_{1-x}Sr_xMnO_3$, x = 0.125
- Intermediate phase T = 140 – 190 K.

Goodenough-Kanamori Rule

- Super-exchange interaction and orbital ordering (Goodenough-Kanamori rule).
- AFM for the same orbital, FM for different orbital.
- Below 150 K, FM state.
- Above 150 K, orbital PM state; super-exchange will be a mixture of FM and AFM.





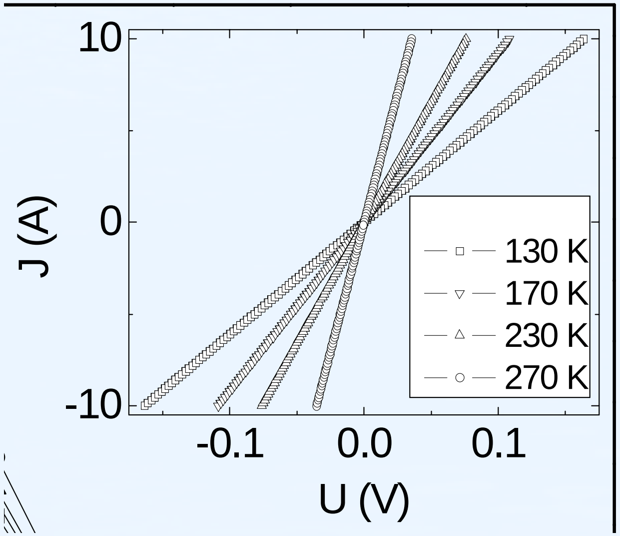
$La_{0.875}Sr_{0.125}MnO_3$

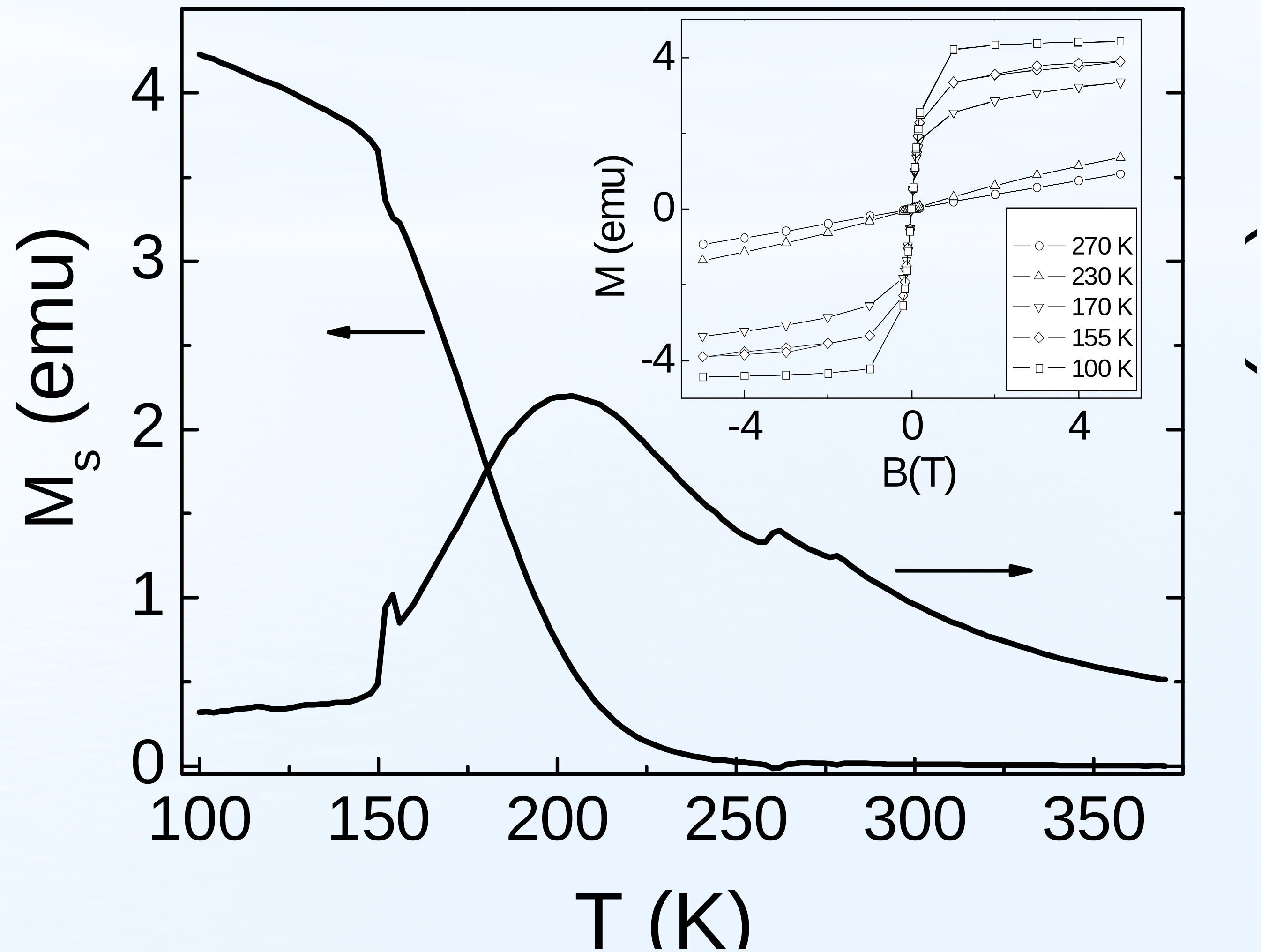
150 K | **190 K**

AFM orbital ordering; FM insulator	**No orbital ordering; mixture of FM metal and AFM/FM insulator**	No orbital and spin ordering; PM insulator charges localized as polarons.

Measurements

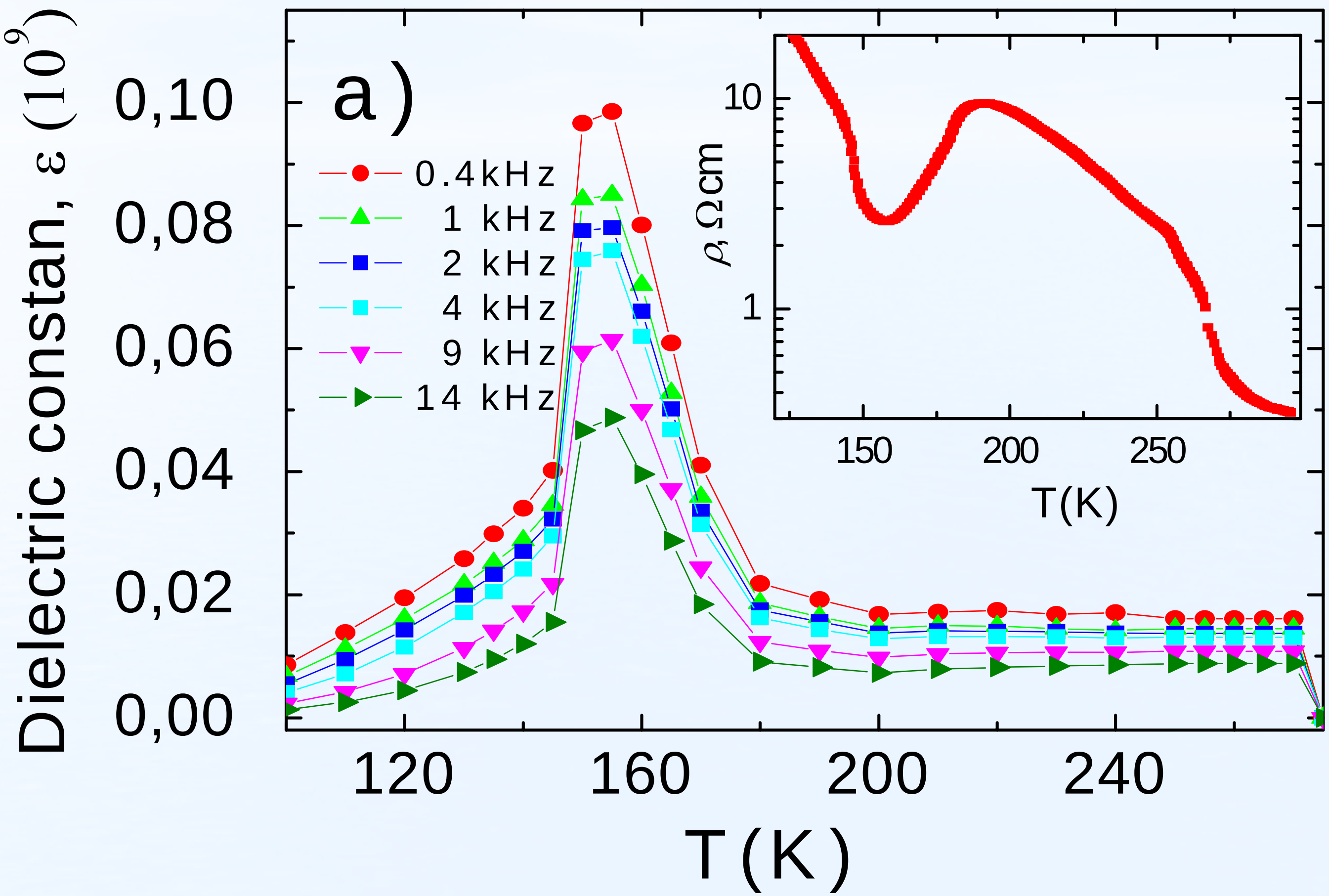
- Single crystal of $La_{0.875}Sr_{0.125}MnO_3$.
- Four-probe measurement of complex dielectric constant with PPMS.
- Applied magnetic field up to 7 T.
- Magnetic measurement with SQUID.
- Contacts are ohmic.





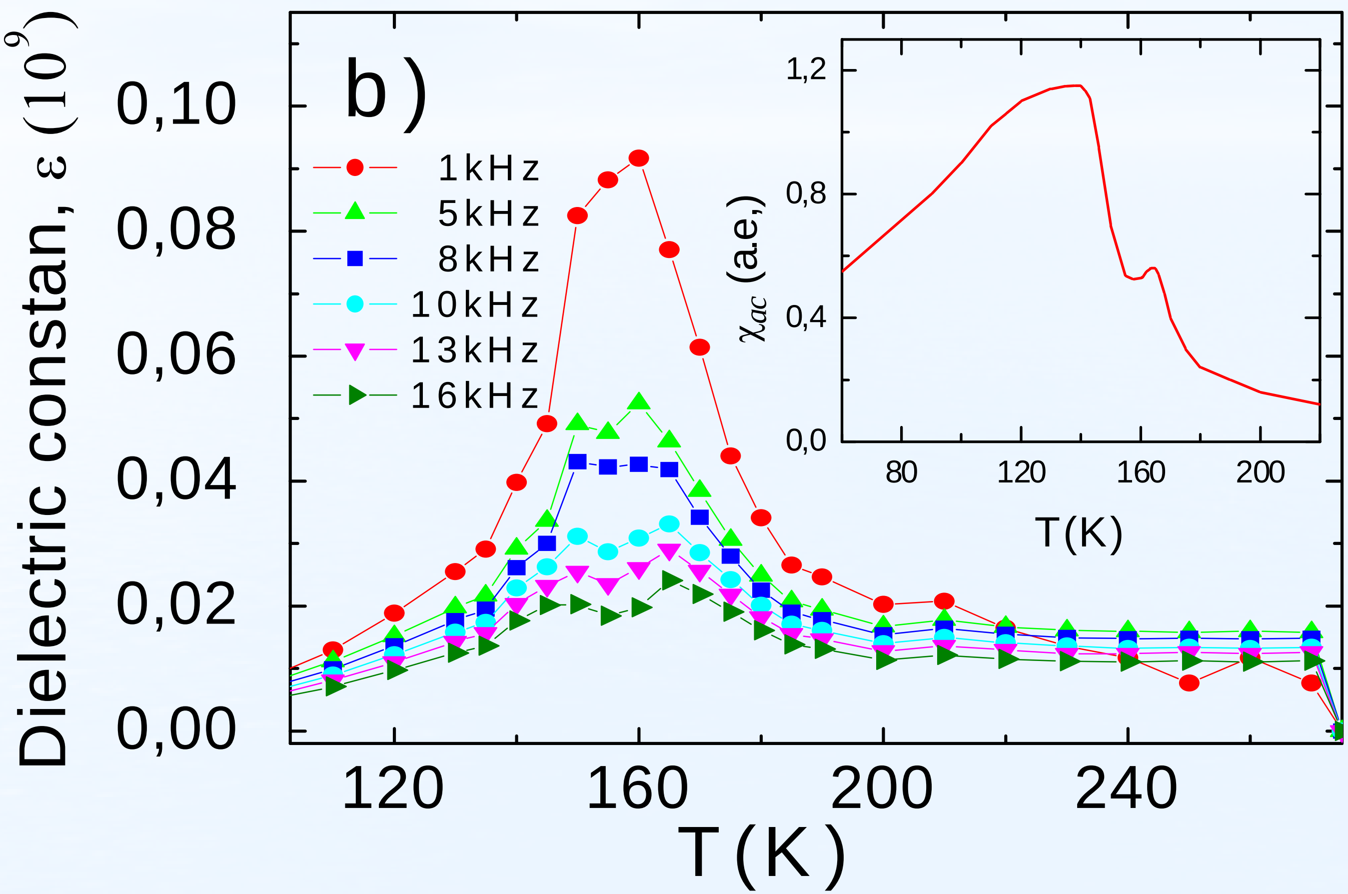
- FM phase partially exists in 150 – 200 K.

Dielectric constant

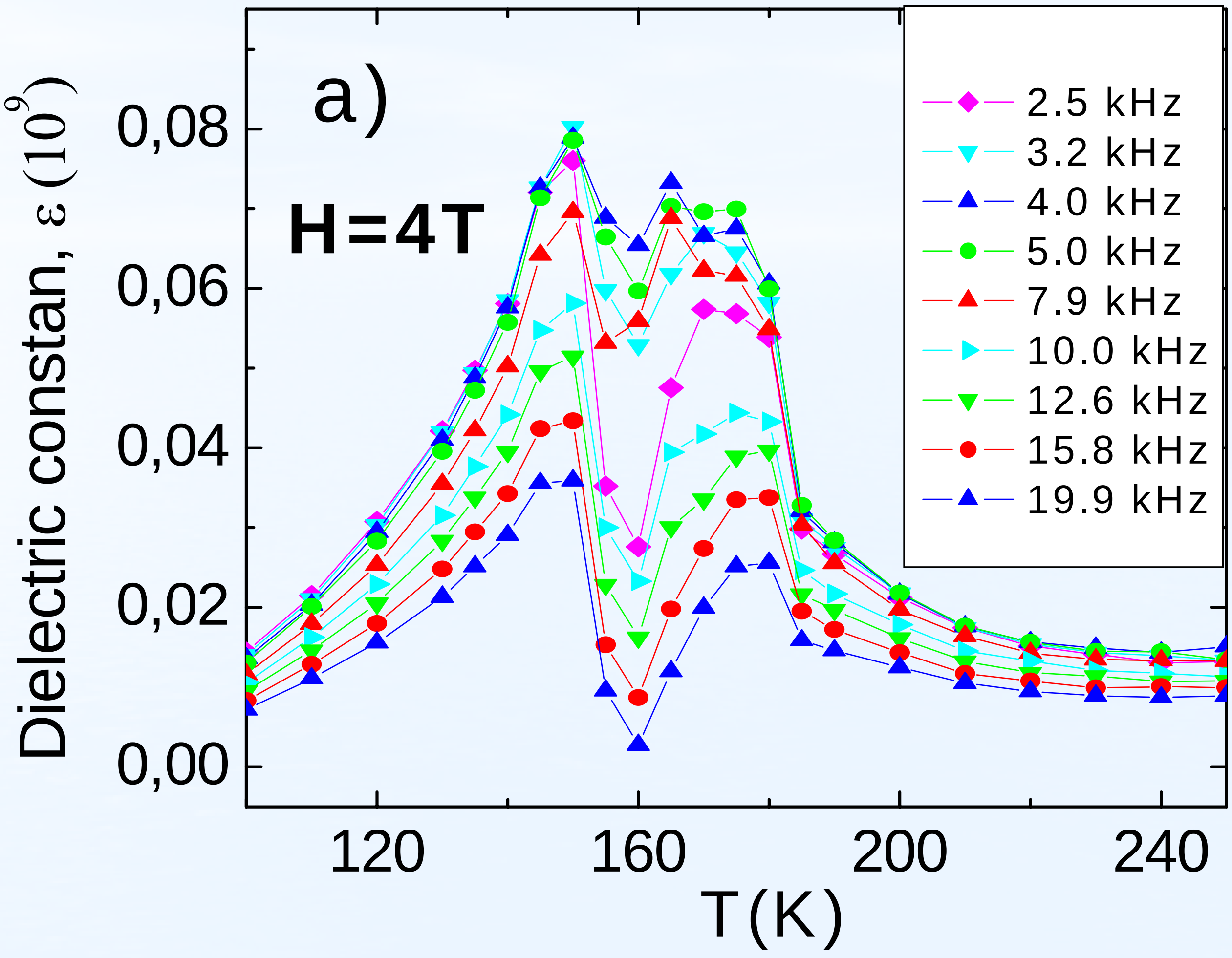


- Zero-field cooling.

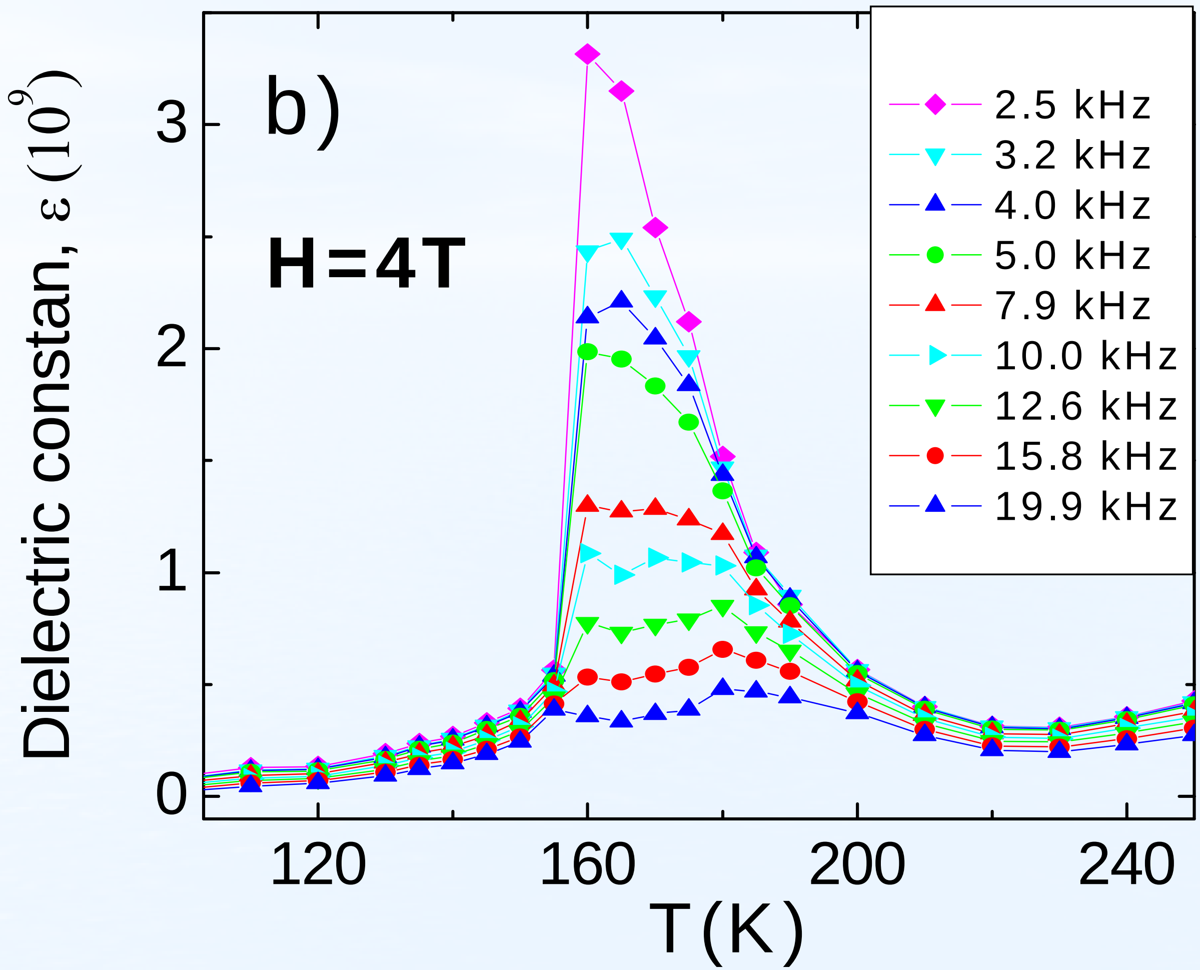
Hysteresis; Spin-Glass Behavior



- Heating after cooling in the field of 2T.

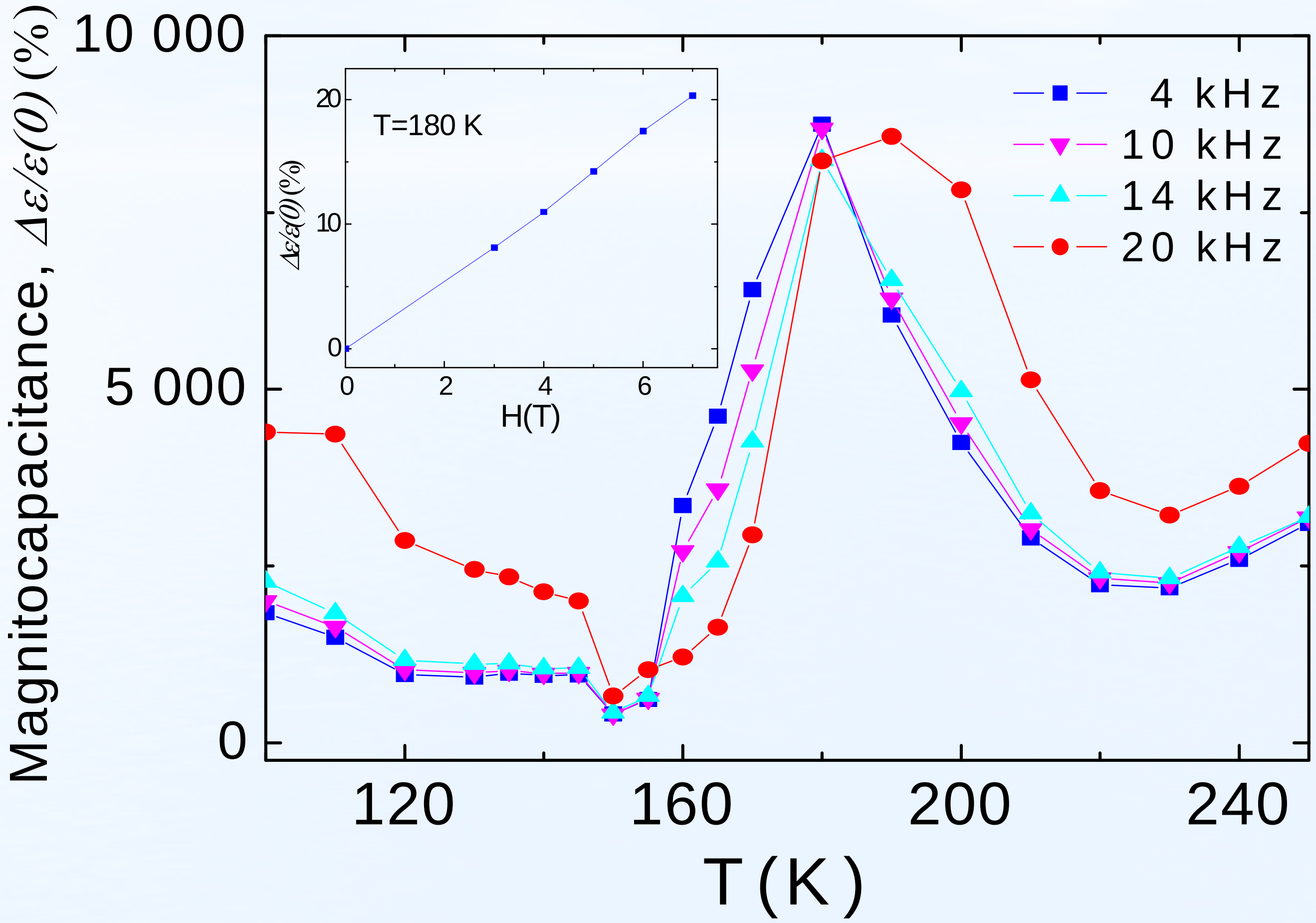


- Cooling in the field of 4T.



- Heating after field cooling in 4T.

Giant Magnetocapacitance



- Magnetocapacitance;

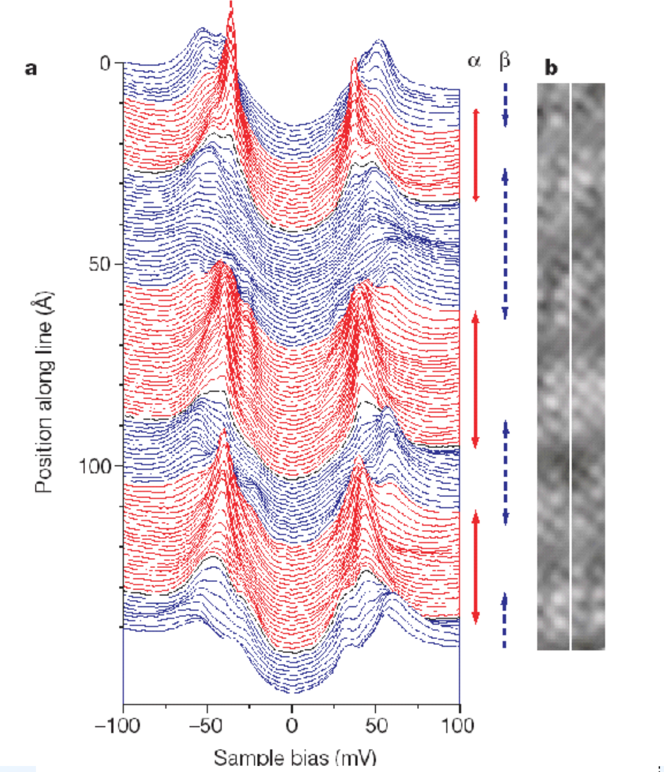
$$MC = \frac{\varepsilon(H) - \varepsilon(0)}{\varepsilon(0)}$$

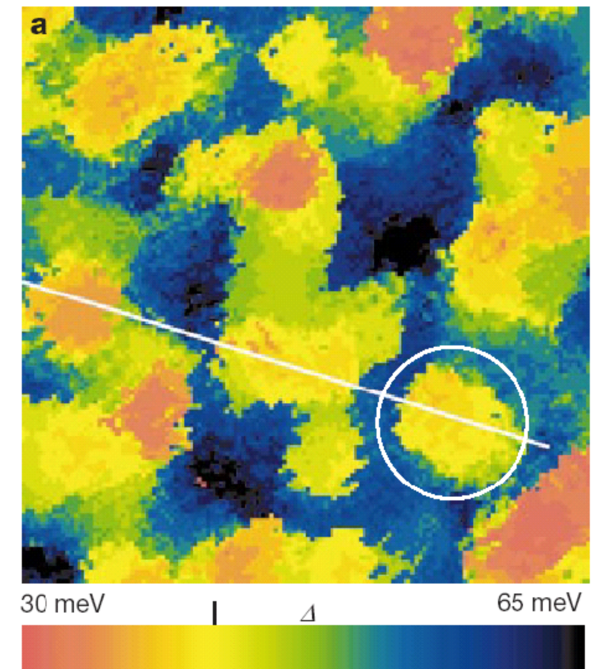
Spatial Inhomogeneity

- A set of very careful STM/STS studies by the group of Seamus Davis reveal electronic inhomogeneity which increases with decreasing charge density.
- The size of the domains is comparable to ξ.
- SC nano-domains with well-defined quasiparticles and domains with pseudo-gap (PG matter).

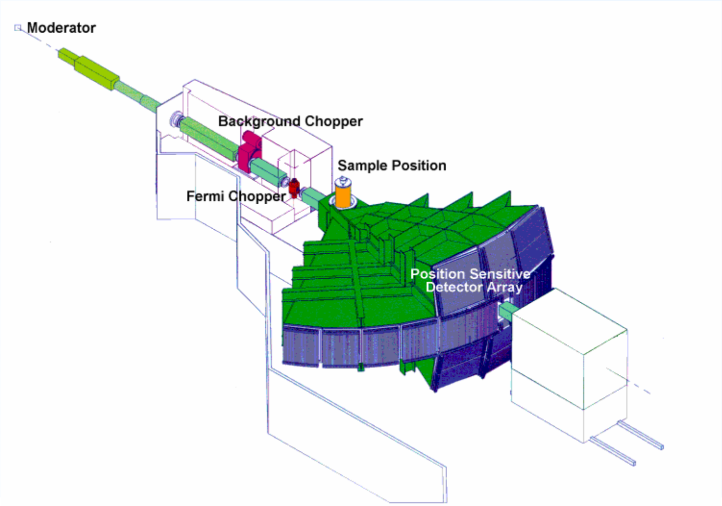
J. C. Davis group

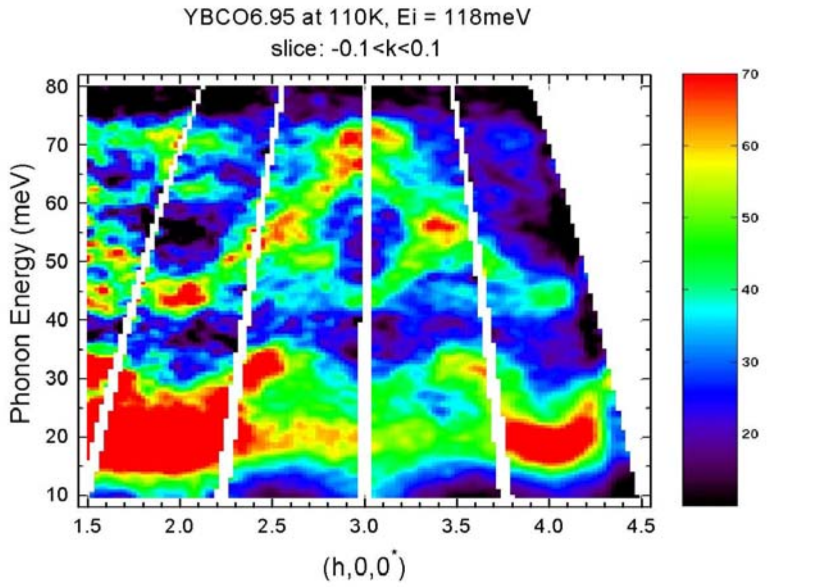
S. H. Pan, et al., *Nature* **413**, 282 (2001).
K. M. Lang, et al., *Nature* **415**, 412 (2002).
K. McElroy, et al., *Nature* **422**, 592 (2003).
K. McElroy, et al., *Science* **309**, 1048 (2005).

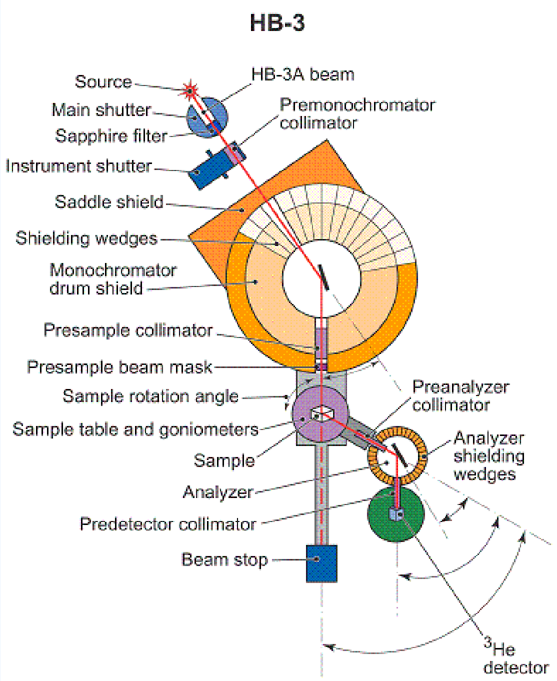




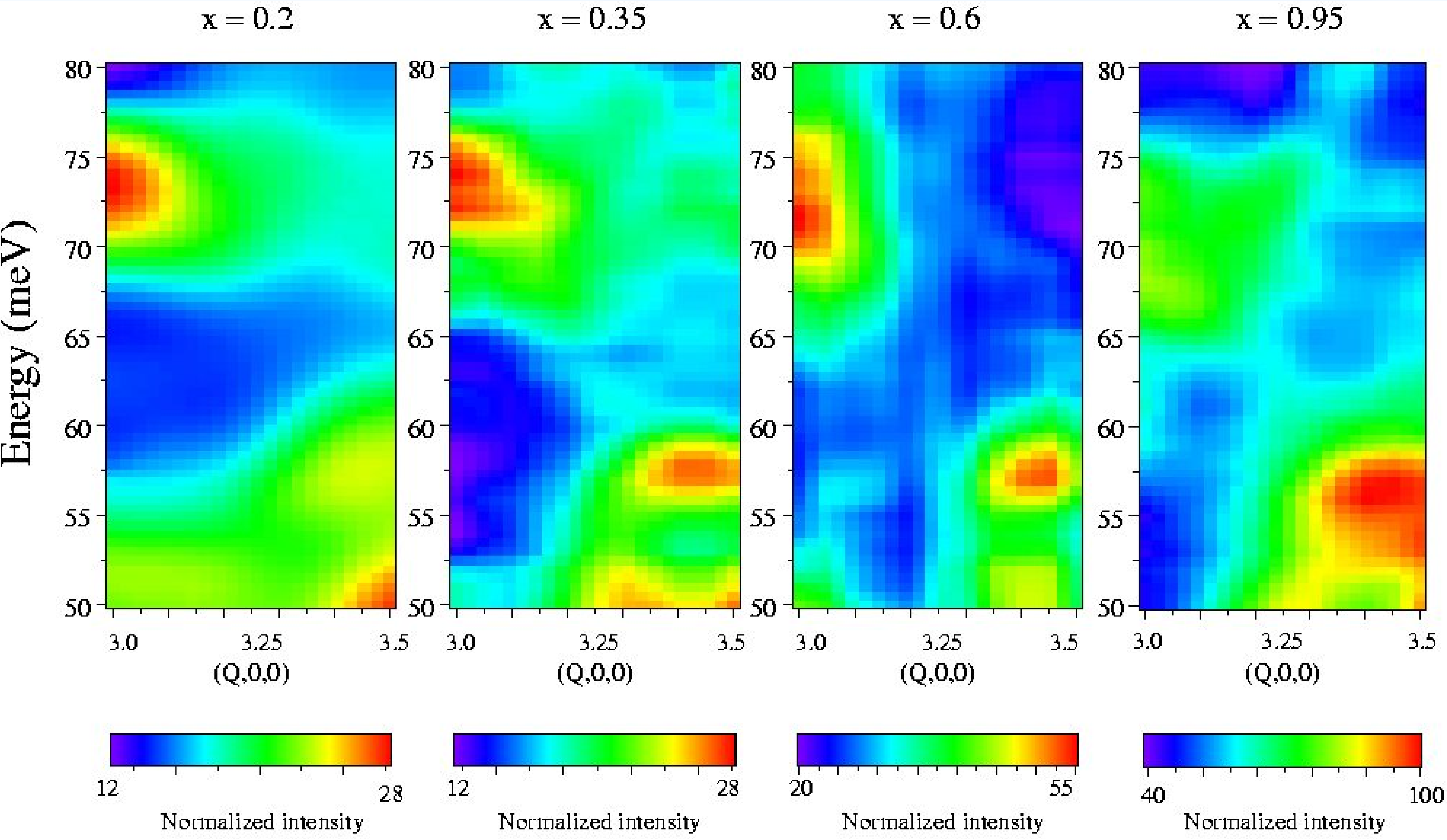
Phonons in YBCO





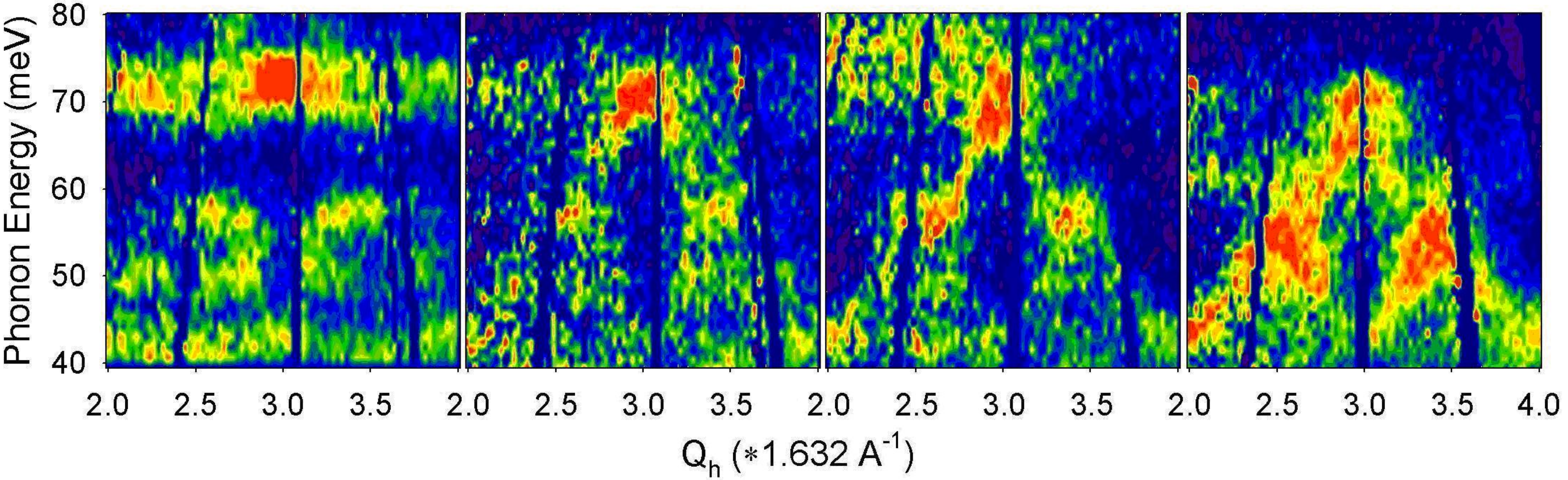


- $YBa_2Cu_3O_{6.95}$, cut along the x-axis, T = 110 K



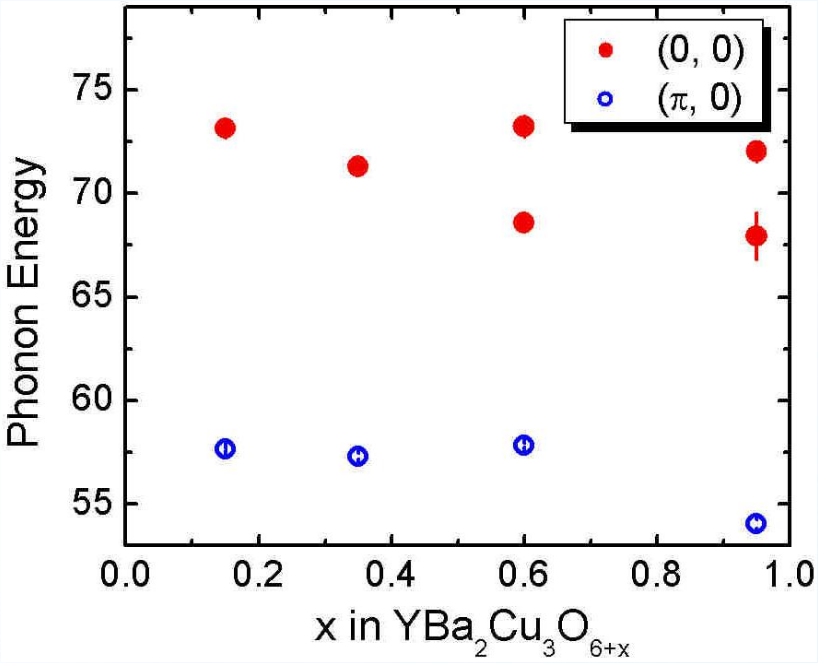
- $YBa_2Cu_3O_{6+x}$; T. Egami, et al. AIP Conf. Proc. **554**, 38 (2001).

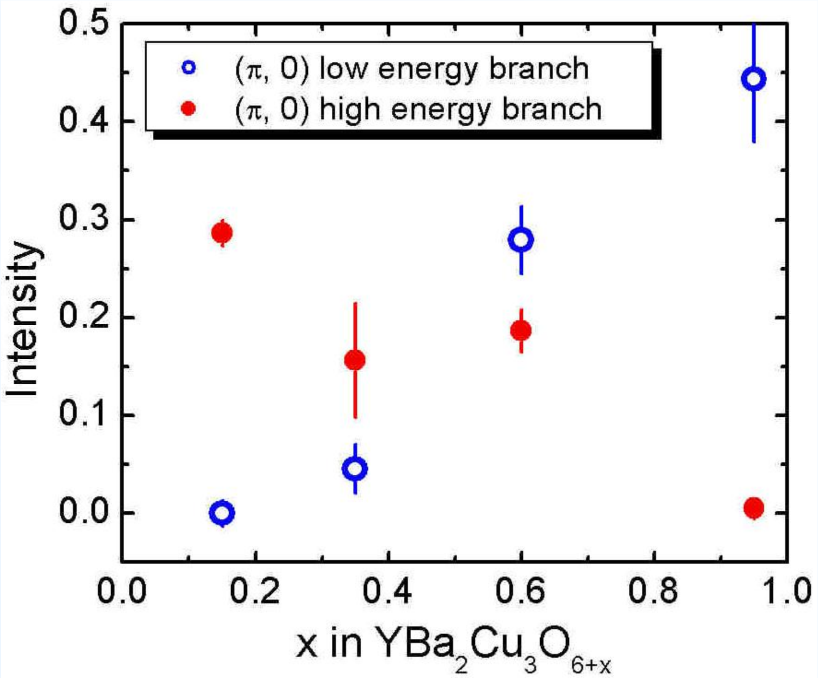
Dependence on Hole Density



6.15 **6.35** **6.6** **6.95**

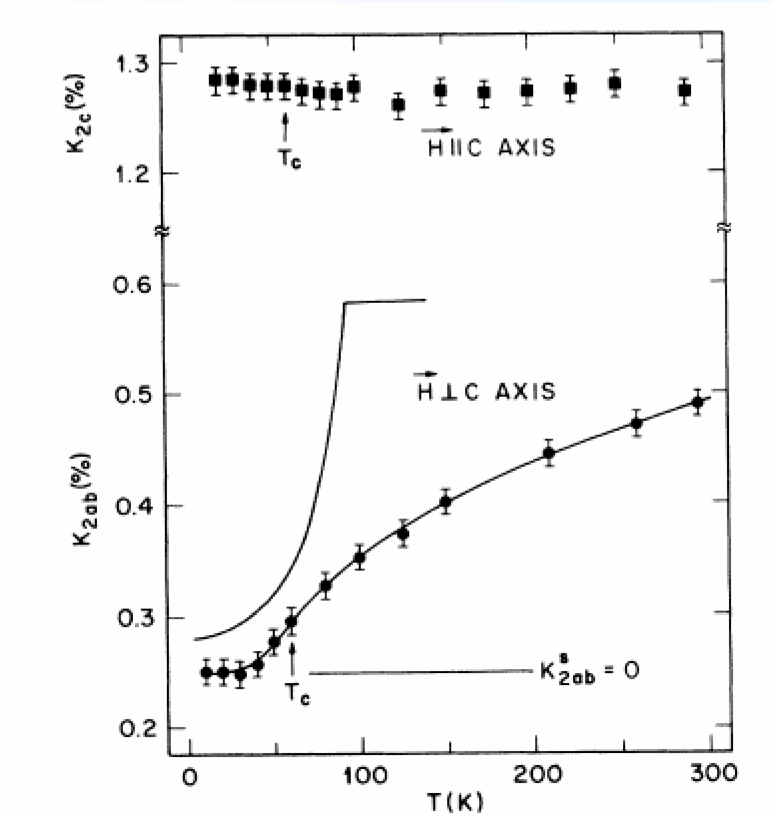
- No dispersion for x = 6.15.
- Not much difference in dispersion from 6.35 to 6.95.
- Intensity at zone-boundary changes.
- Since 6.35 is tetragonal this is not the consequence of anisotropy.





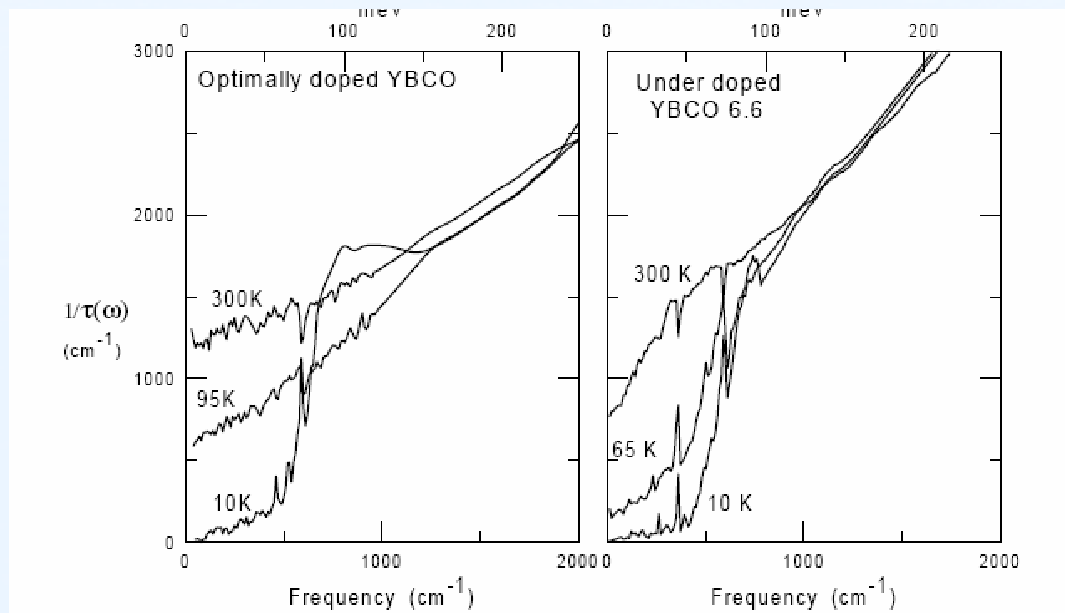
- The magnitude of softening is independent of *x*, but the intensity of the softened branch increases with increasing *x*.
- At $x = 6.15$ the intensity is due to the apical mode.
- The increase has to be due to the local modes.
- Softened (SC) and unsoftened (AFM) domains?

Pseudo-Gap State

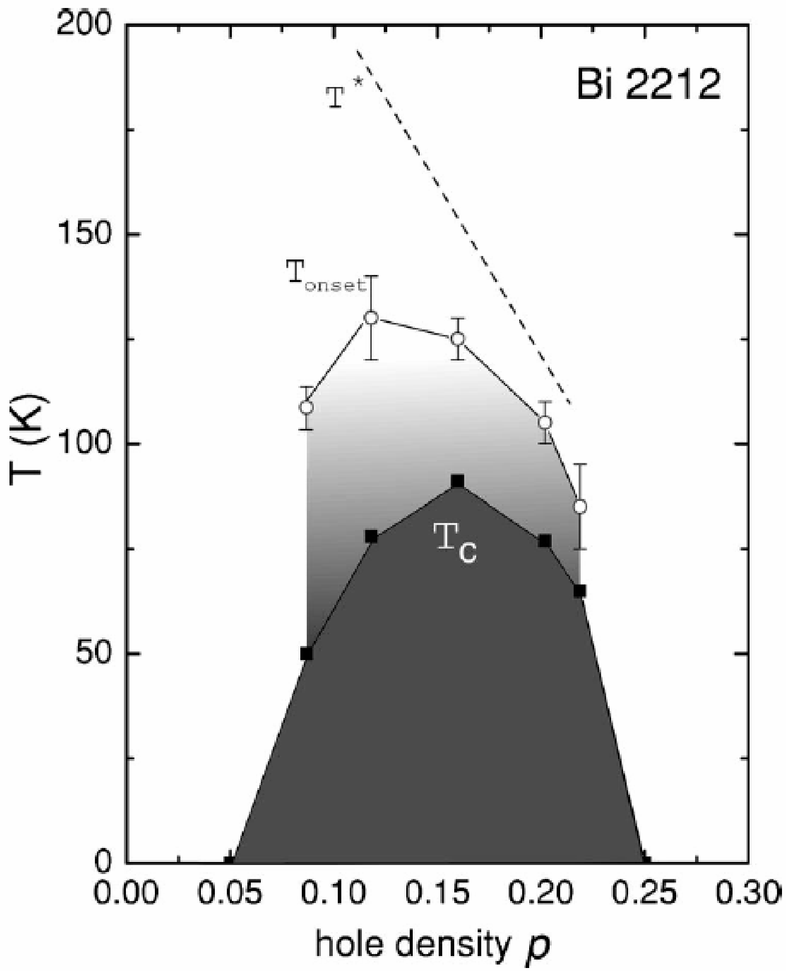


R. E. Walstedt et al., *Phys. Rev. B* **41**, 9574 (1990).

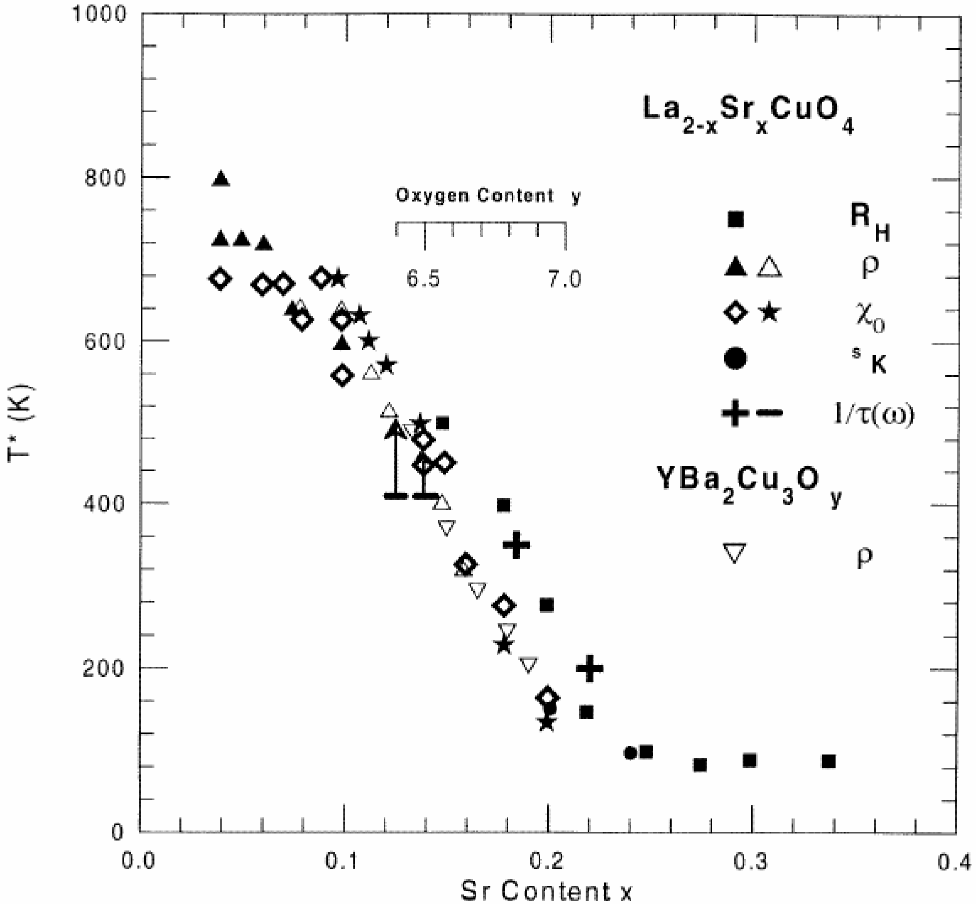
- Observed first by NMR.
- Clearly seen by IR, ARPES and tunneling probes including STS.
- Indirectly seen by resistivity, Hall effect, thermal conductivity.



T. Timusk and B. Statt, *Rep. Prog. Phys.* **62**, 61 (1999).



N. P. Ong, *Phys. Rev. B* **73,** 024510 (2006)



T. Timusk and B. Statt, *Rep. Prog. Phys.* **62**, 61 (1999).

Nature of the PG State

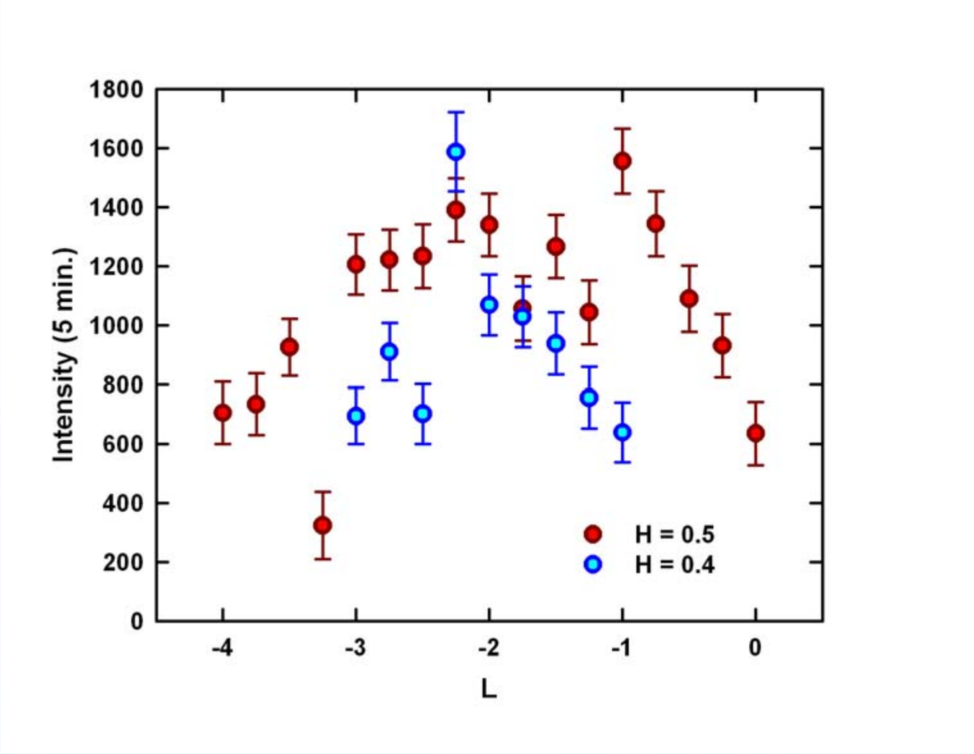
- Competing order
  - Magnetic ordering (local)
  - Orbital magnetism (flux state, *d*-*d*-wave)
  - Charge ordering
- Pre-formed pair
  - Local BCS pairing
  - Bipolarons

Neutron Scattering from YBCO6.6 Single Crystal

- $YBa_2Cu_3O_{6.6}$ single crystal (25g). T_C = 60 K.
- Neutron elastic scattering, spin unpolarized.
- SPINS, NIST; HB1-A, HFIR, ORNL.
- Temperature dependent scattering.
- Green phase (Y_2BaCuO_5) ~ 10%, T_N = 16K.
- Close to Q = 0, almost no effect of phonons.

CuO_2 Bilayer

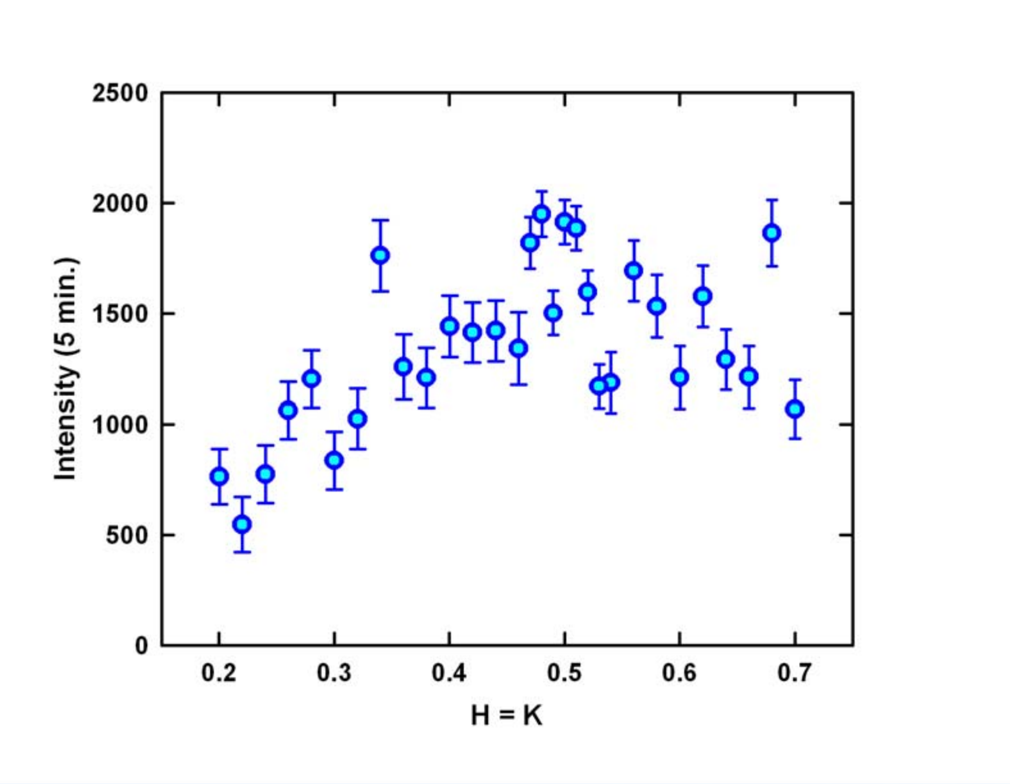
- CuO_2 bilayer with the separation of 3.2 Å, corresponding to L = 3.6.
- A peak at L = 1.8 most likely due to AFM spin correlation in the bilayer.
- Similar L-dependence seen for the neutron resonance peak.
- Energy resolution 0.5 meV.



I(20K) – I(270K) for (H, H, L) scan. A peak at L = -2 most likely due to bilayer AFM correlation.

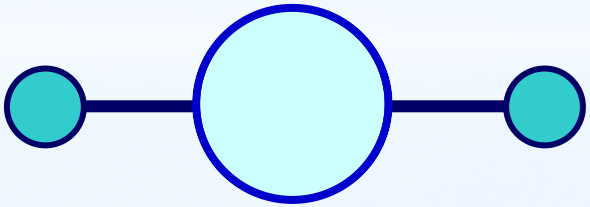
Spin-Glass-Like Behavior

- Broad in H; in-plane correlation length 10 ~ 15 Å.
- If cluster AFM, the temperature dependence should be super-paramagnetic 1/T behavior.
- Likely to involve positive J as well.



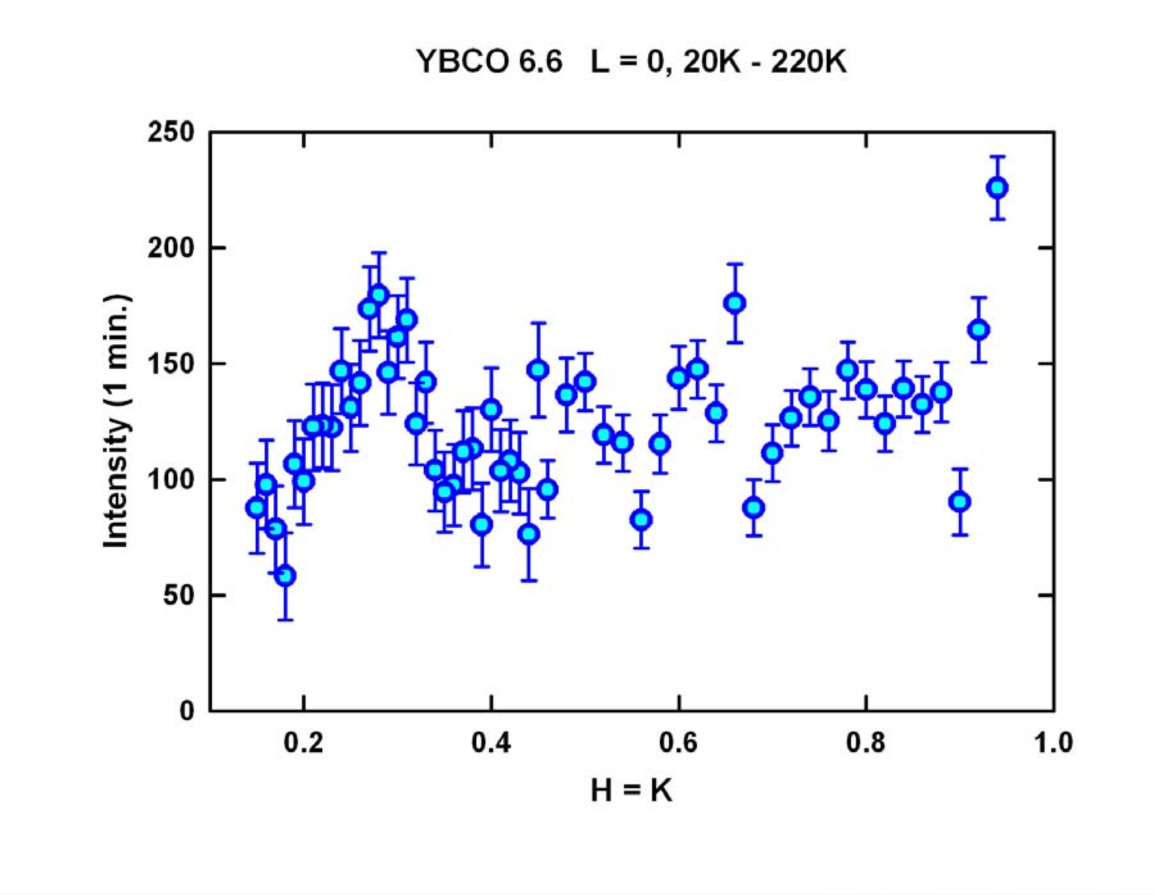
Spin-Glass and Variation in J

- The presence of spin-glass state implies that some *J*'s are positive.
- Vick Emery predicted it, when hole resides on oxygen, not in the Z-R singlet state.
- In manganites double-exchange results in positive *J*.
- *t-J* model is insufficient.



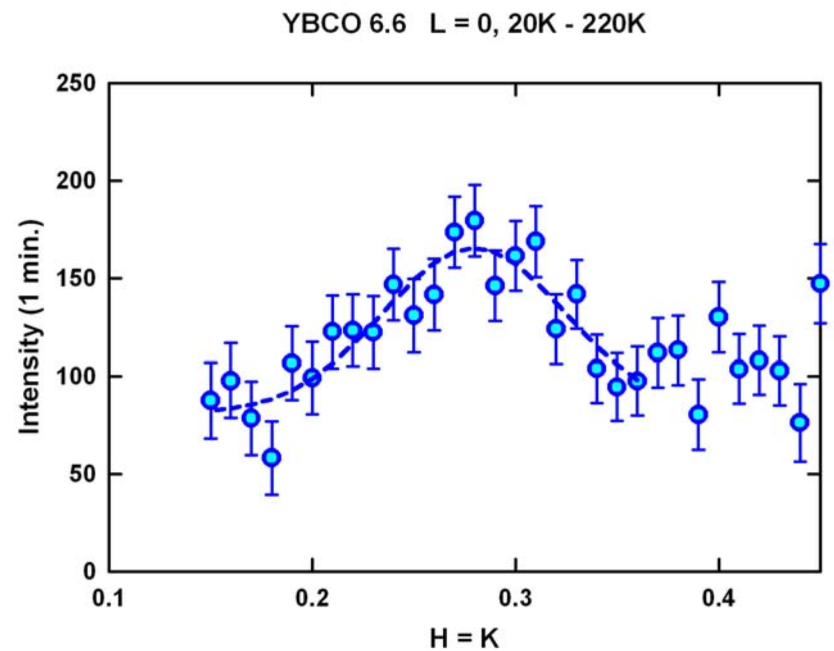
L = 0 Scan

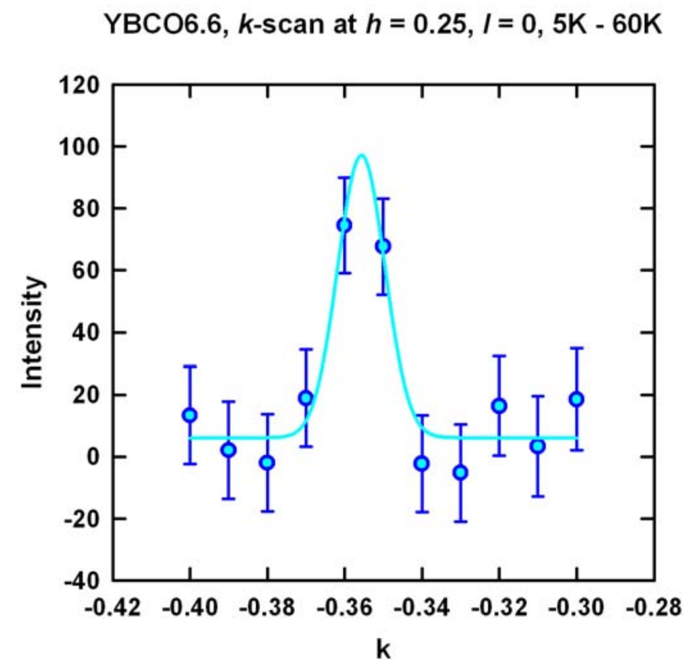
- Complex behavior with a peak around (0.28, 0.28, 0) ~ (1/4, 1/4, 0).
- Significant background; very small at low Q.



Peak at H = K = 0.28

- Peak height comparable to the powder AFM peak of the included green phase (Y_2BaCuO_5, ~ 10%).
- Diffuse peak; short-range order with the coherence of ~ 30 Å.
- Not phonons (~ Q^2).
- Estimated to be 5% in volume if we assume $S = 1/2$.



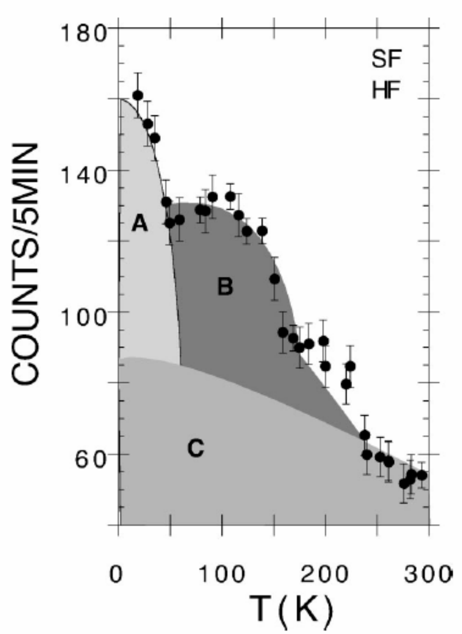


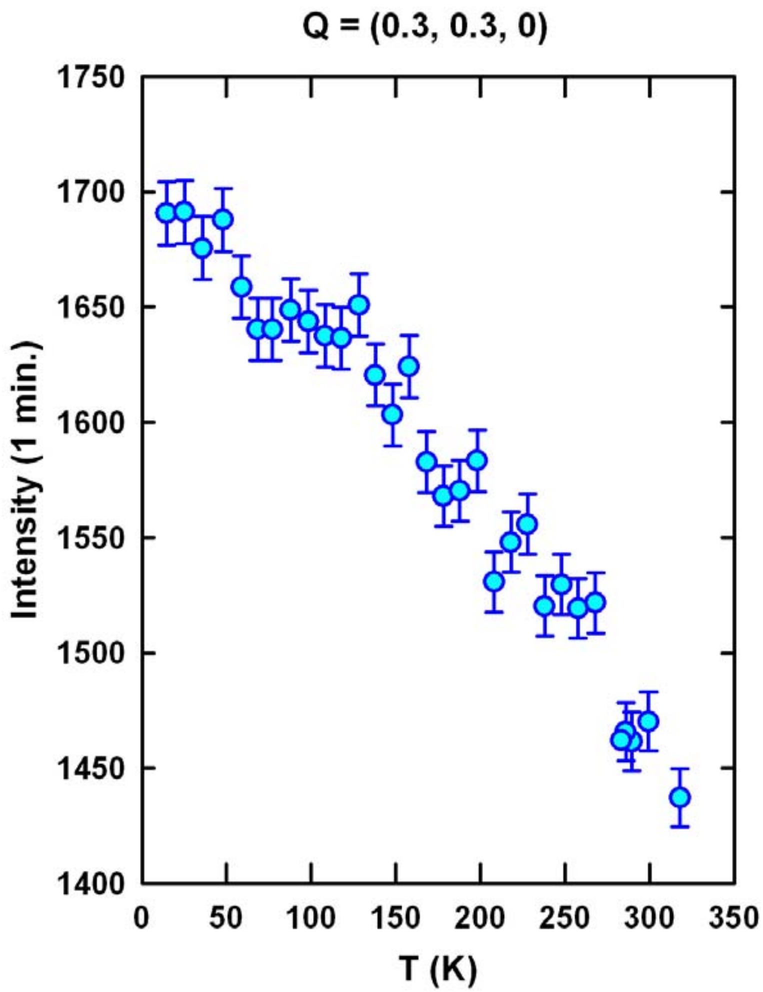
Temperature Dependence

- Decreases with increasing T; not phonons.
- Some anomaly near $T_C = 60K$?
- Some change near $T_{PG} \sim 250K$??

Peak at (0.5, 0.5, 0) in YBCO6.6.

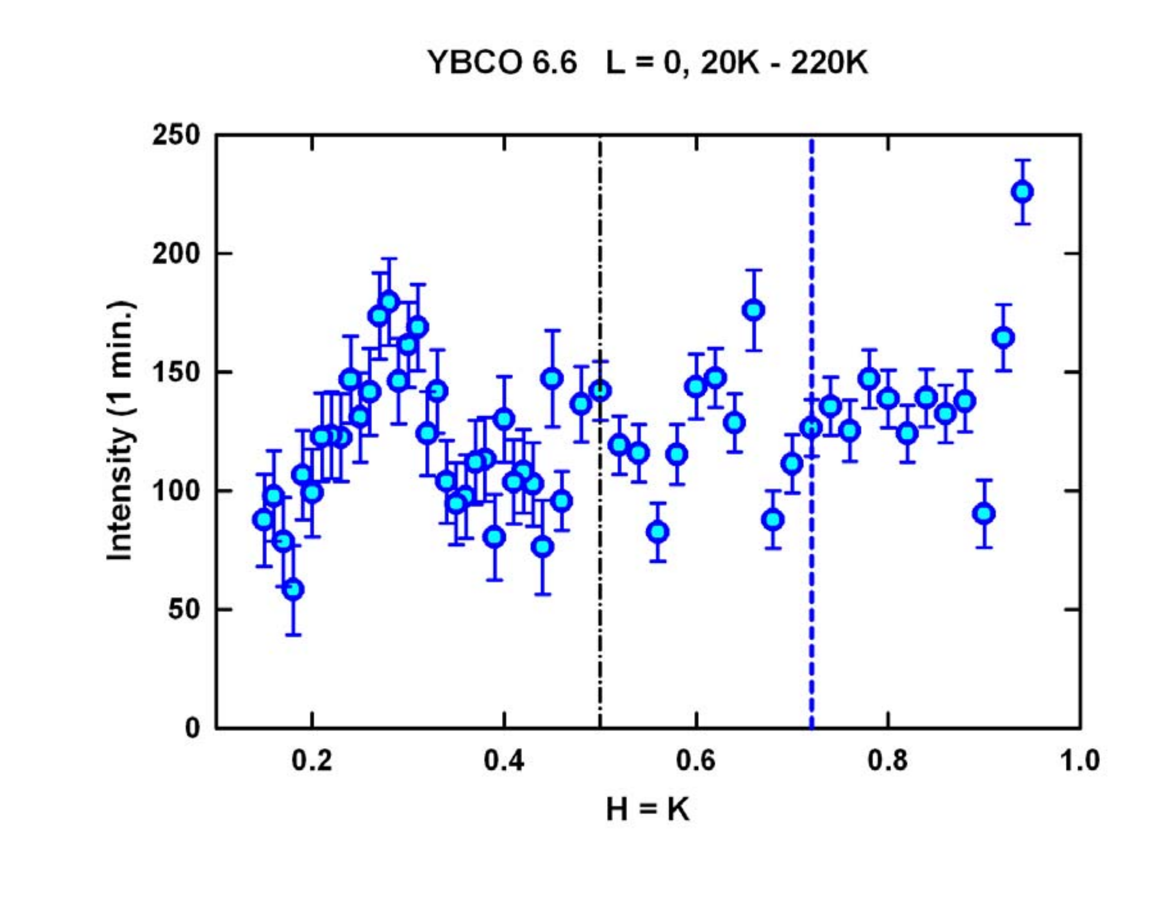
H. A. Mook, *et al*, *PRB* **66,** 144513 (2002).





Nature of the Local Ordering

- Spin-glass behavior?
- No symmetry about (0.5, 0.5, 0); spins not centered on Cu or O. Hybridized Cu-O orbitals not included in the *t-J* model?
- The peak at (0.28, 0.28, 0) ~ (¼, ¼, 0) could be related to the $2\sqrt{2}\times2\sqrt{2}$ electronic medium-range order.
- Related to the pseudo-gap phase?



Intermediate Phase in Doped Mott-Hubbard Insulator

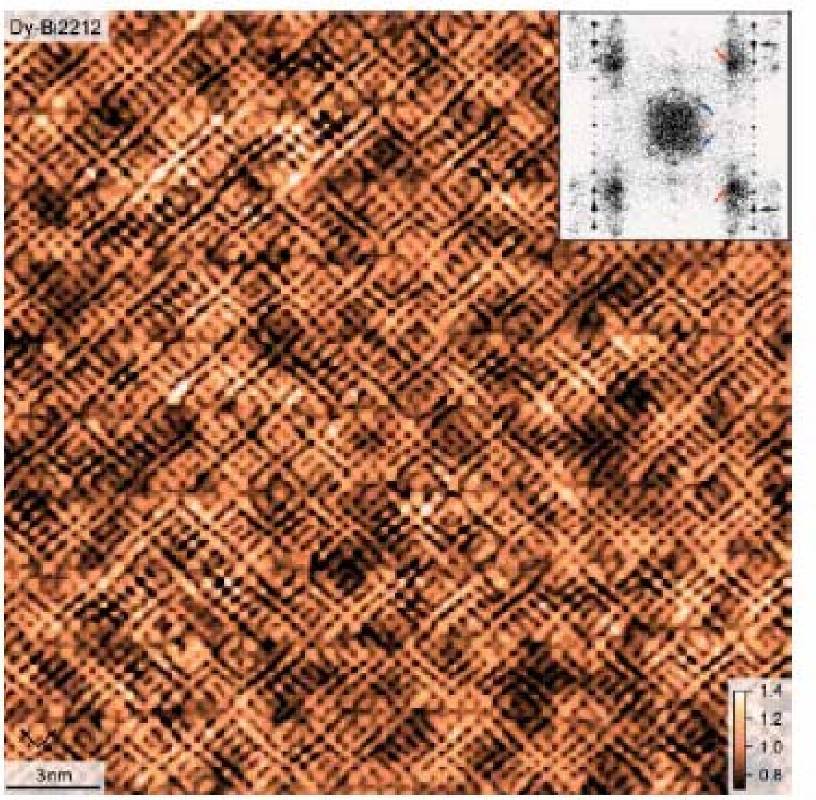
- The transition from a doped Mott-Hubbard state to a Fermi-liquid could induce electronic phase separation. Because of the Coulomb repulsion spin and charge will self-organize themselves to form an intermediate state.

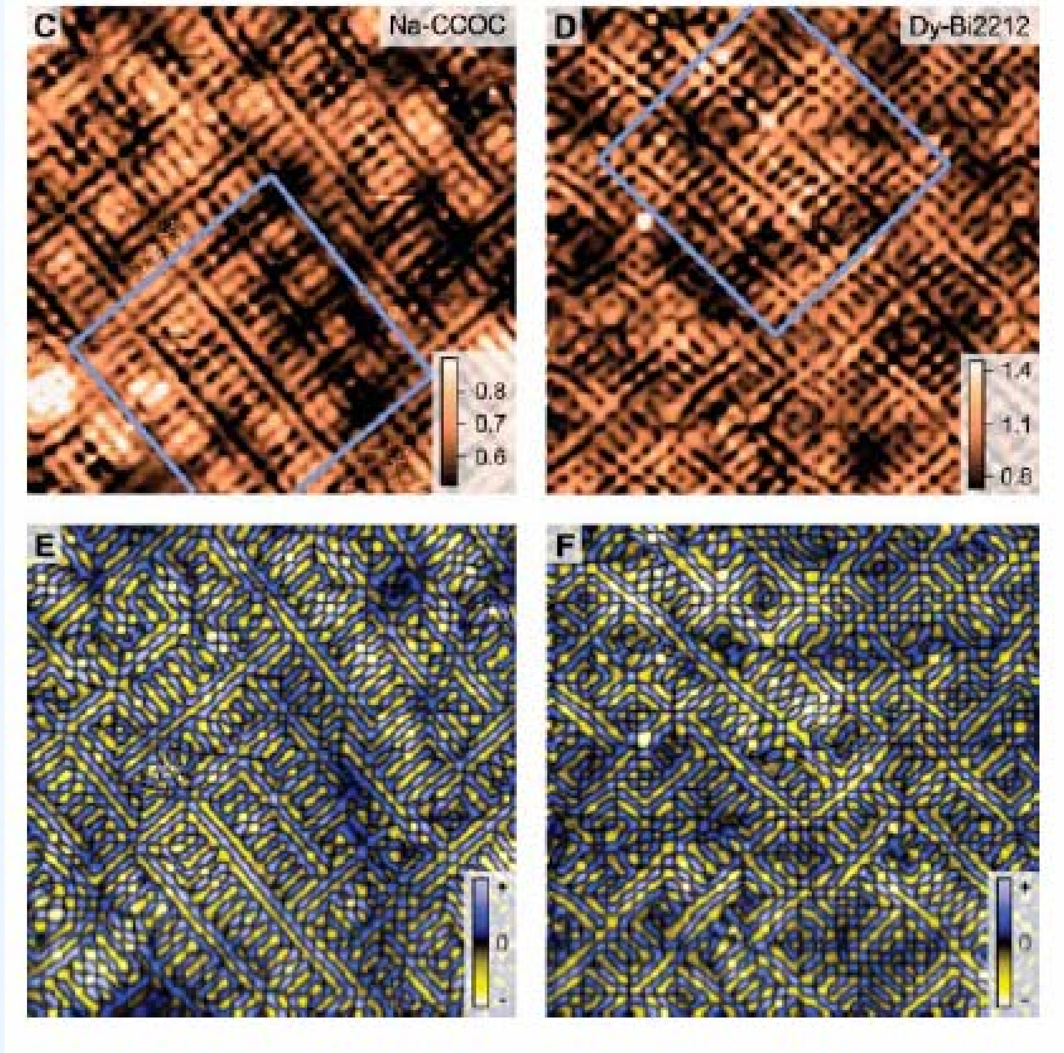
- The stripe state is a possible intermediate state, but the one-dimensional nature of the stripes is incompatible with the strongly two-dimensional character of the Cu-O plane.

- Two-dimensional intermediate phase is a possibility.

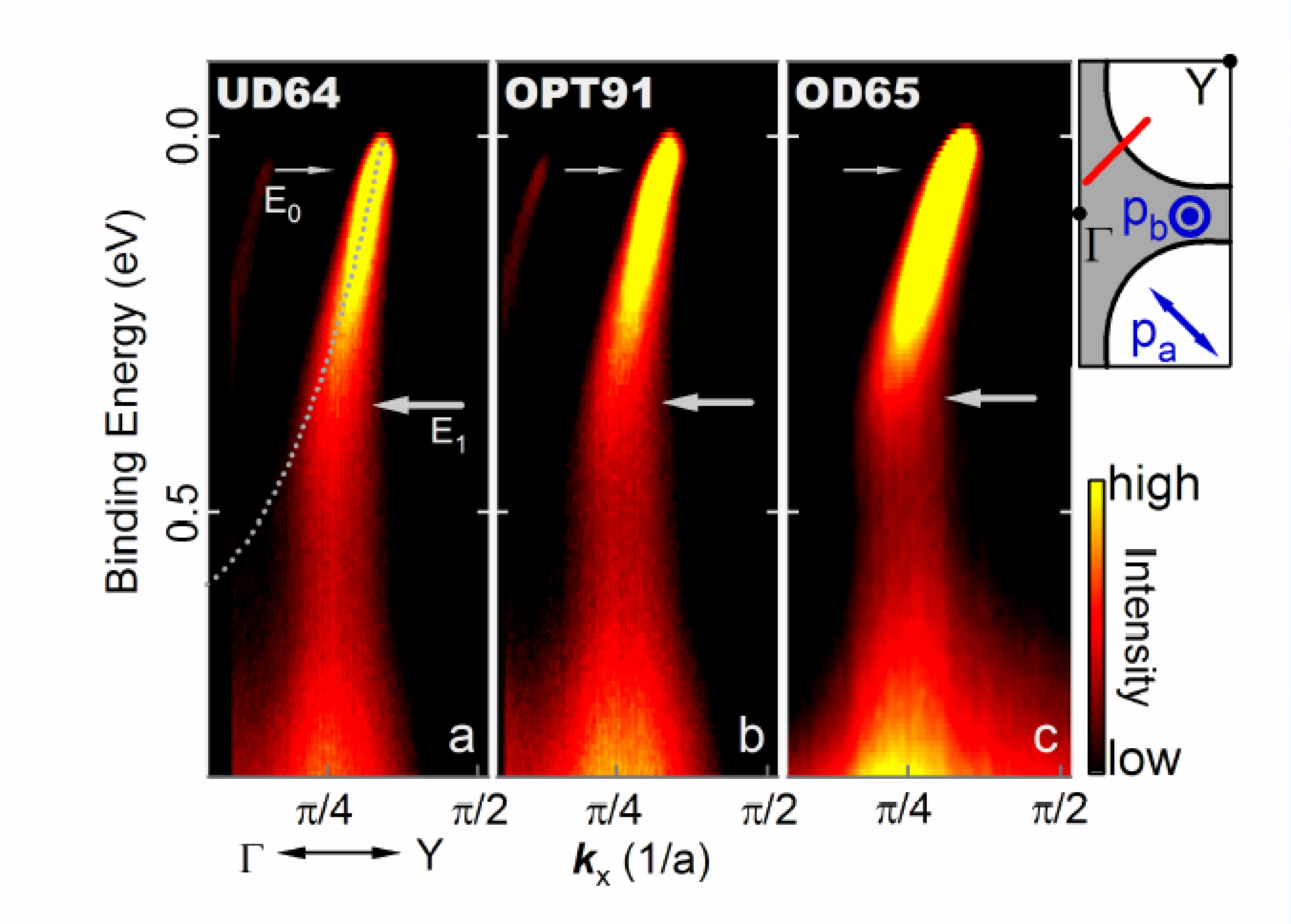
Checkerboard

- Hole on oxygen, 4 x 4 structure.....



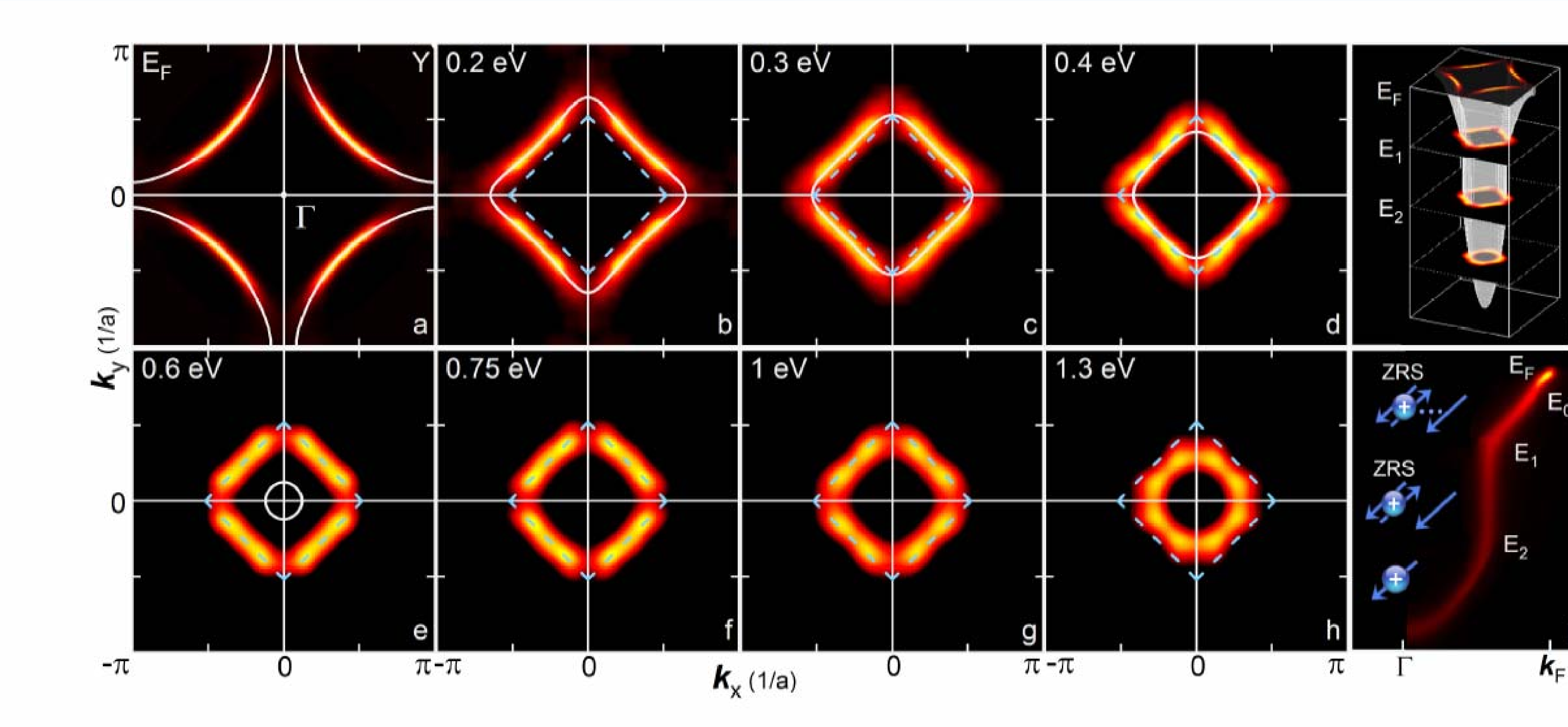


Y. Kohsaka, et al., *Science* **315,** 1380 (2007)



J. Graf, G.-H. Gweon, K. McElroy, S. Y. Zhou, C. Jozwiak, E. Rotenberg, *cond-mat/0607319*

- Gap-like feature from -0.4 to – 1 eV, regardless of doping.

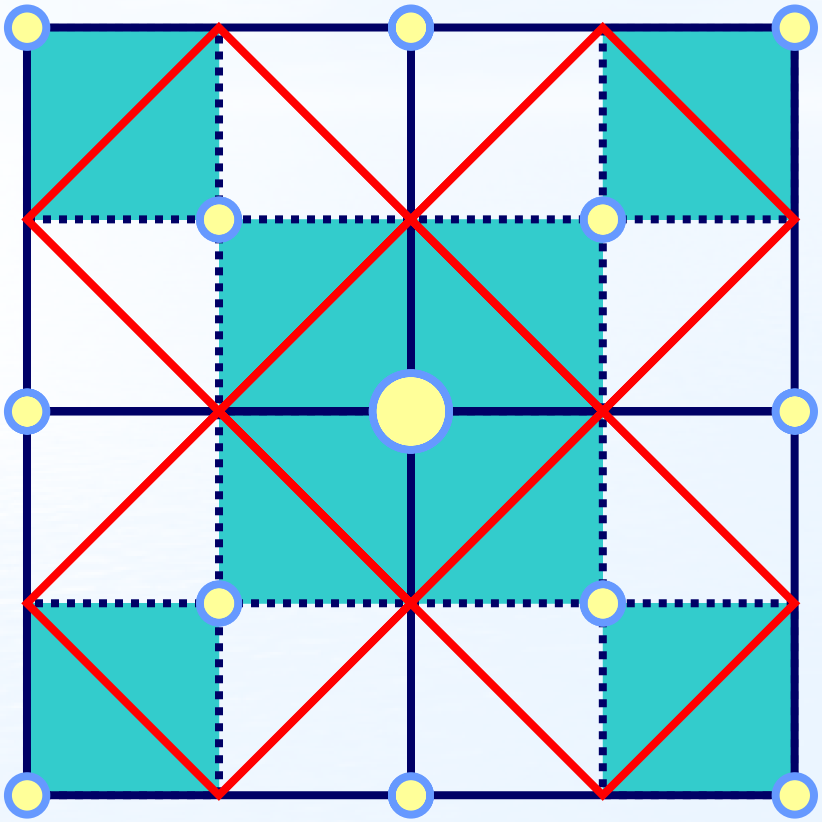


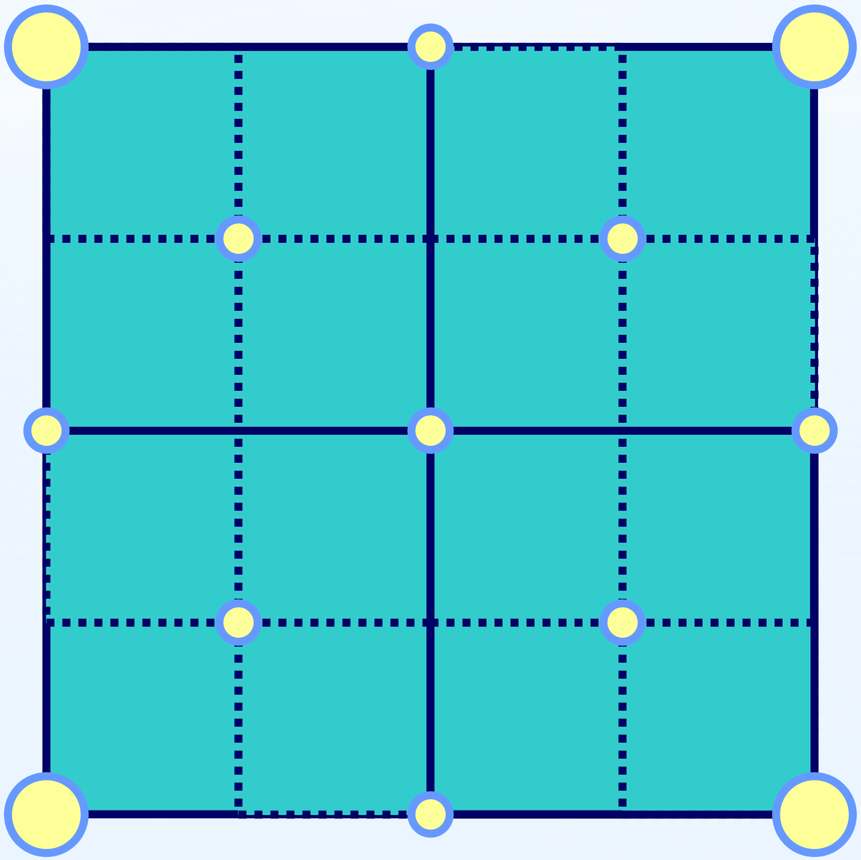
J. Graf, G.-H. Gweon, K. McElroy, S. Y. Zhou, C. Jozwiak, E. Rotenberg, *cond-mat/0607319*

- Brillouin zone (?) by 8 fold ($2\sqrt{2}\times 2\sqrt{2}$).

Superlattice

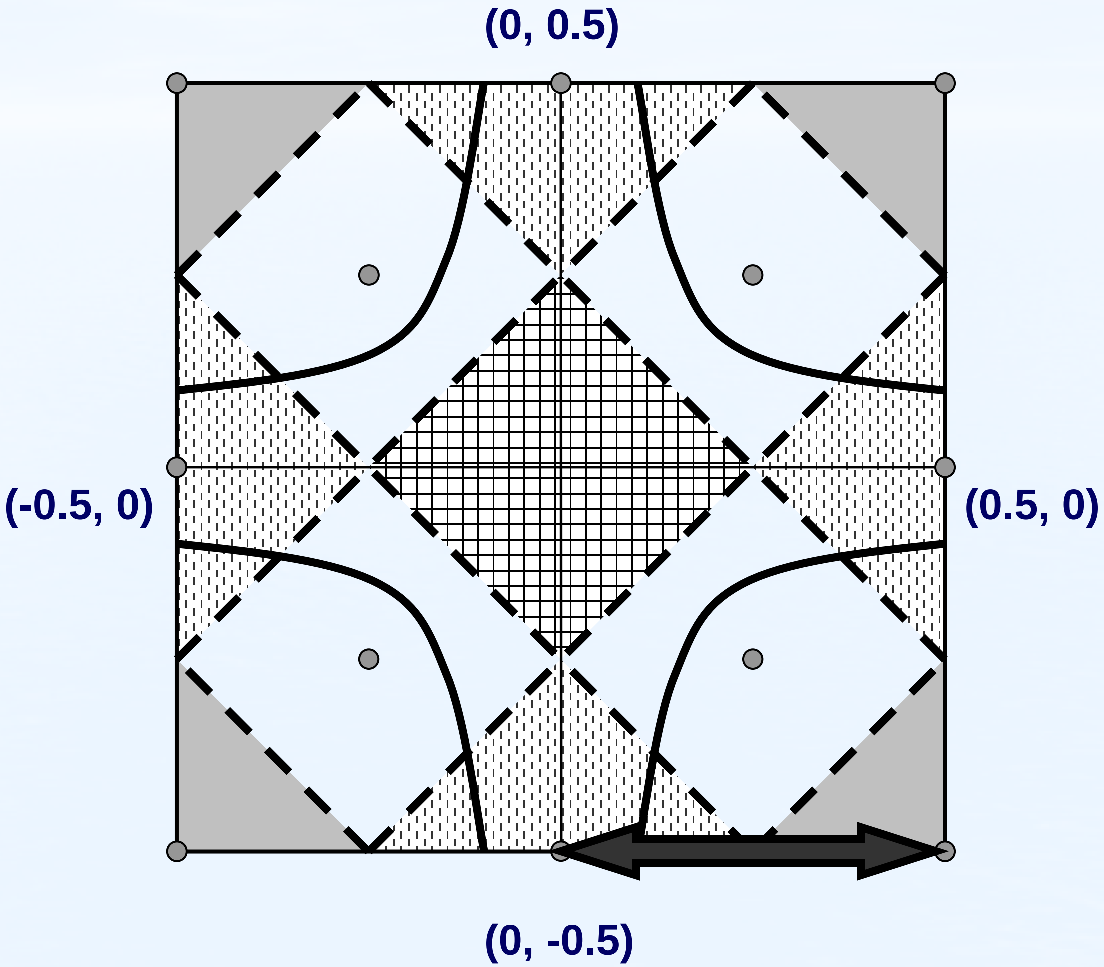
- ($\pi/2$, $\pi/2$) superlattice.



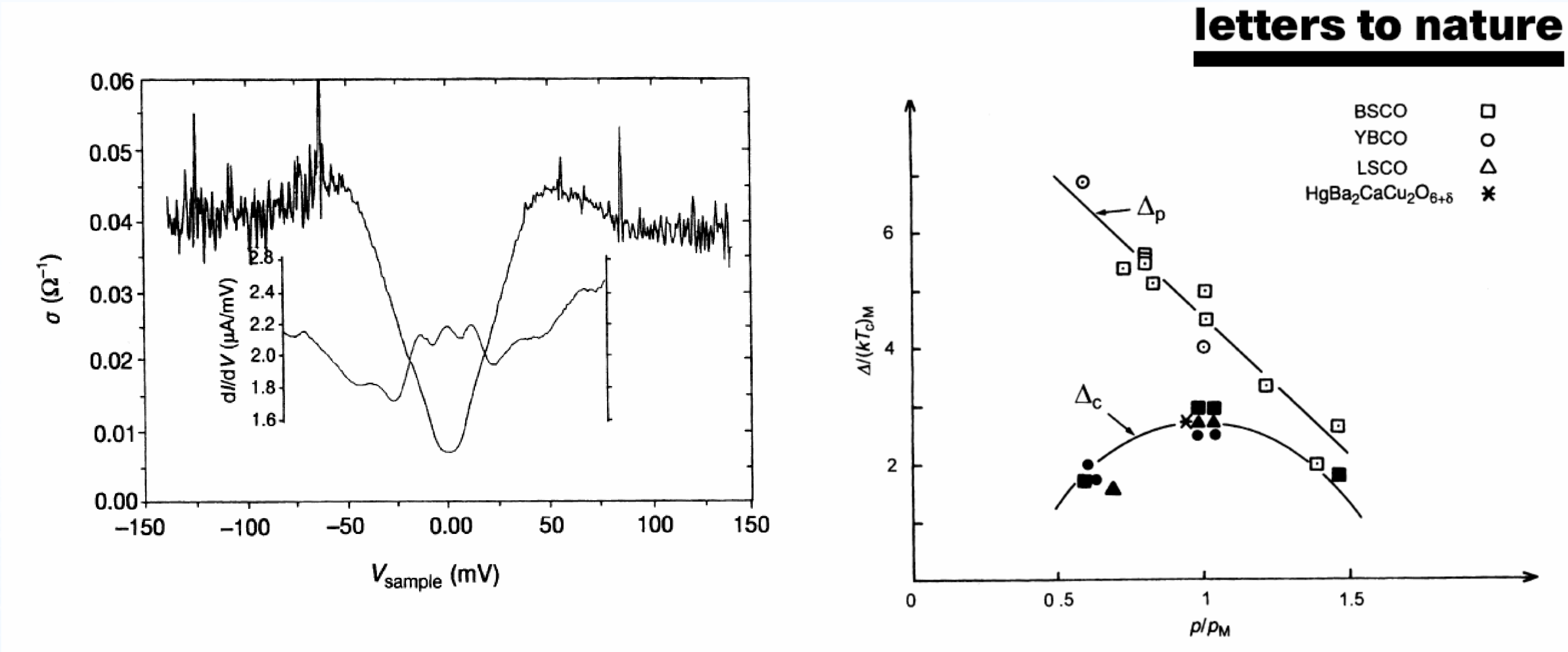


Sub-Brillouin Zones

- Nodal and anti-nodal particles in different sub-B. Z.
- Anti-nodal particles with more Cu character, and nodal particle with oxygen character.
- Anti-nodal states may be localized.



Two Gaps

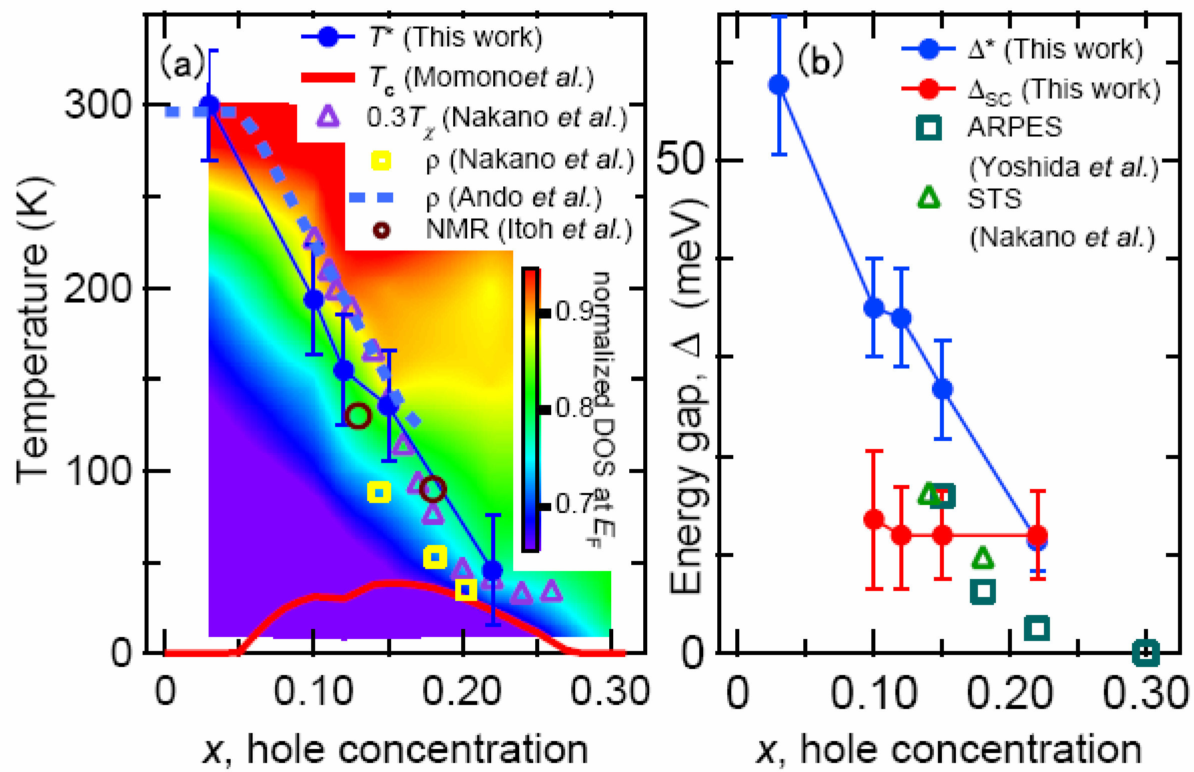


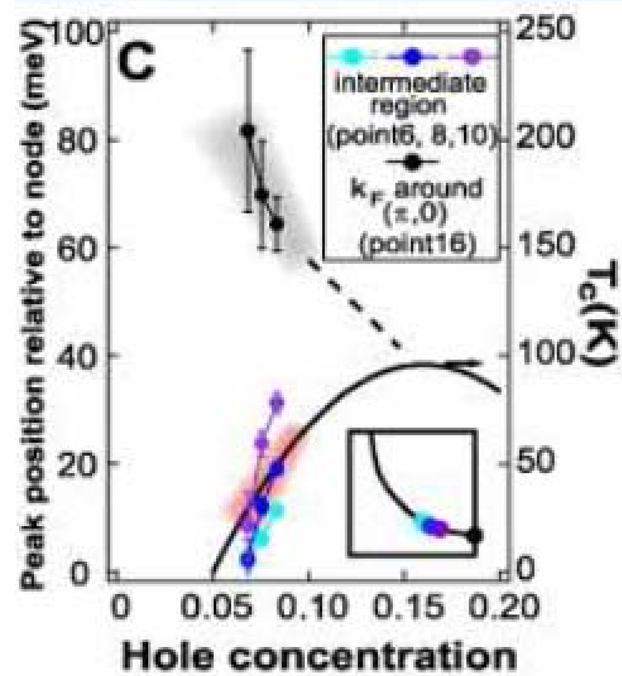
G. Deutscher, *Nature* **397,** 410 (1999)

- Coherence peak by Andreev reflection follows T_C, while the pseudogap follows T_{PG}.

$$\frac{2\Delta_{SC}}{kT_C} \approx \frac{2\Delta_{PG}}{kT_{PG}} \approx 4$$

Two Gaps



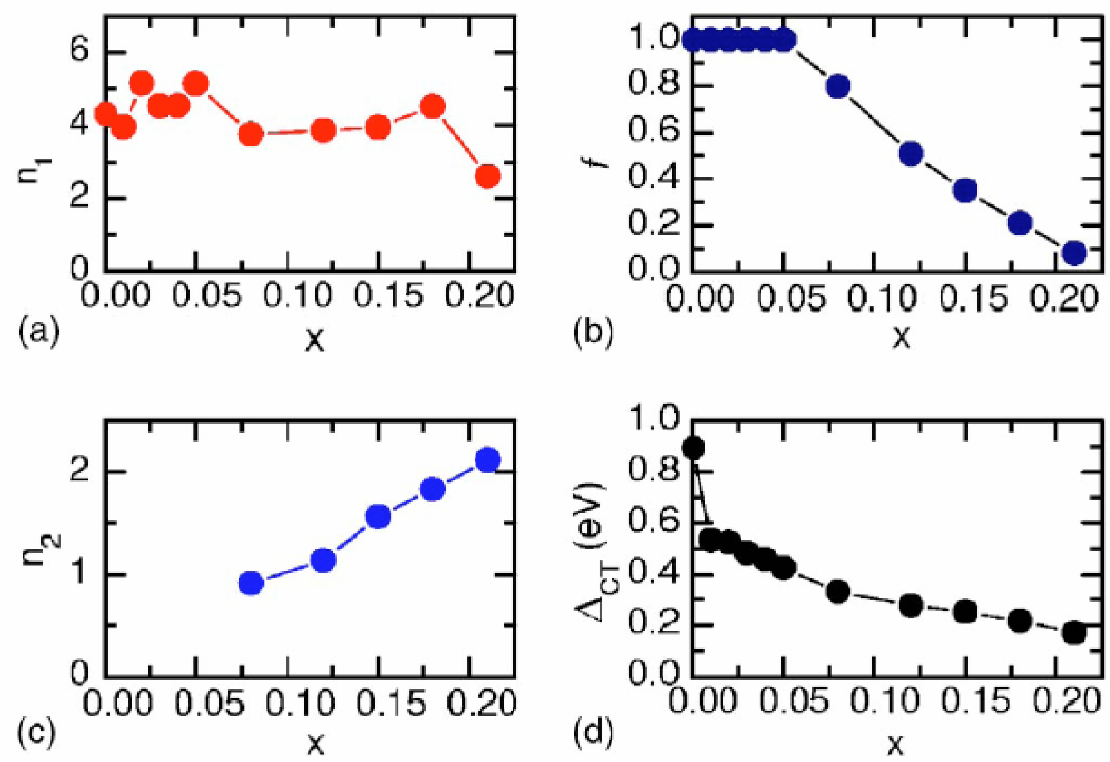


M. Hashimoto, T. Yoshida, K. Tanaka, A. Fujimori, M. Okusawa, S. Wakimoto, K. Yamada, T. Kakeshita, H. Eisaki and S. Uchida, *Phys. Rev. Lett.*, to be published

K. Tanaka, W. S. Lee, D. H. Lu, A. Fujimori, T. Fujii, Risdiana, I. Terasaki, J. D. Scalapino, T. P. Devereaux, Z. Hussain and Z.-X. Shen, *Science*, **314,** 1910 (2006).

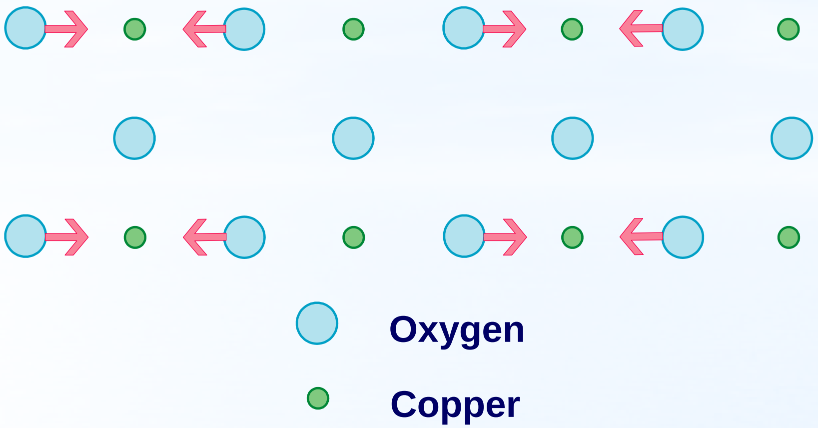
Charge Nature of the PG State

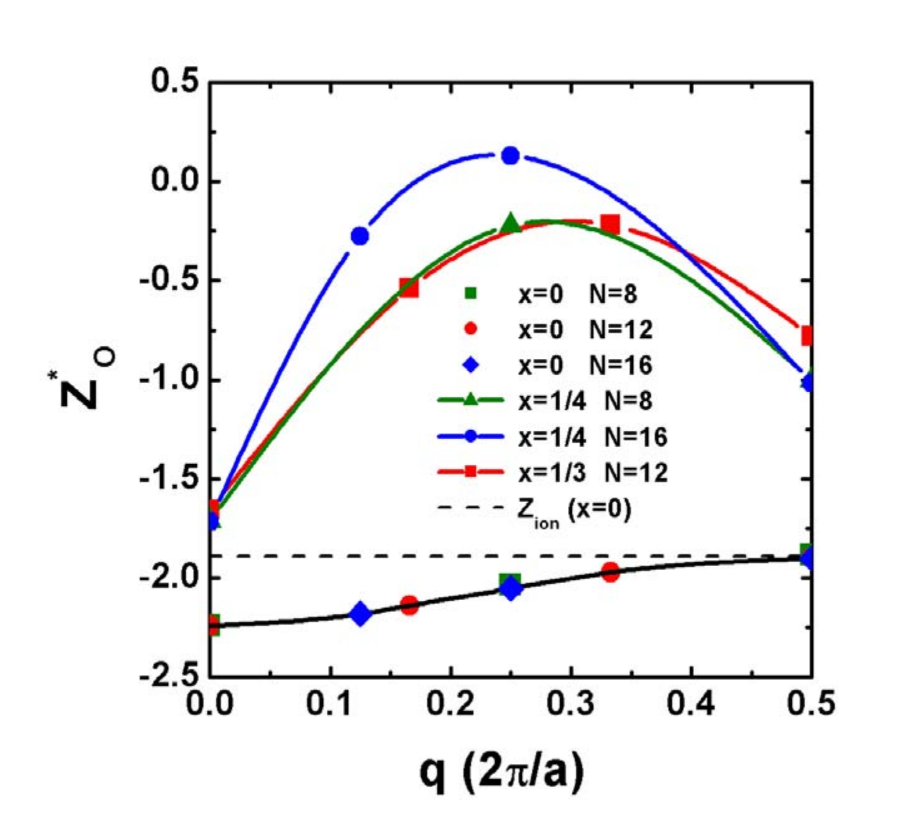
- Two kinds of carriers.
- The one associated with PG involves charge excitation gap.
- Agrees with the metal-insulator transition seen under high magnetic field.



S. Ono, S. Komiya and Y. Ando, *PRB* **75,** 024515 (2007)

Cu-O Bond-stretching Mode



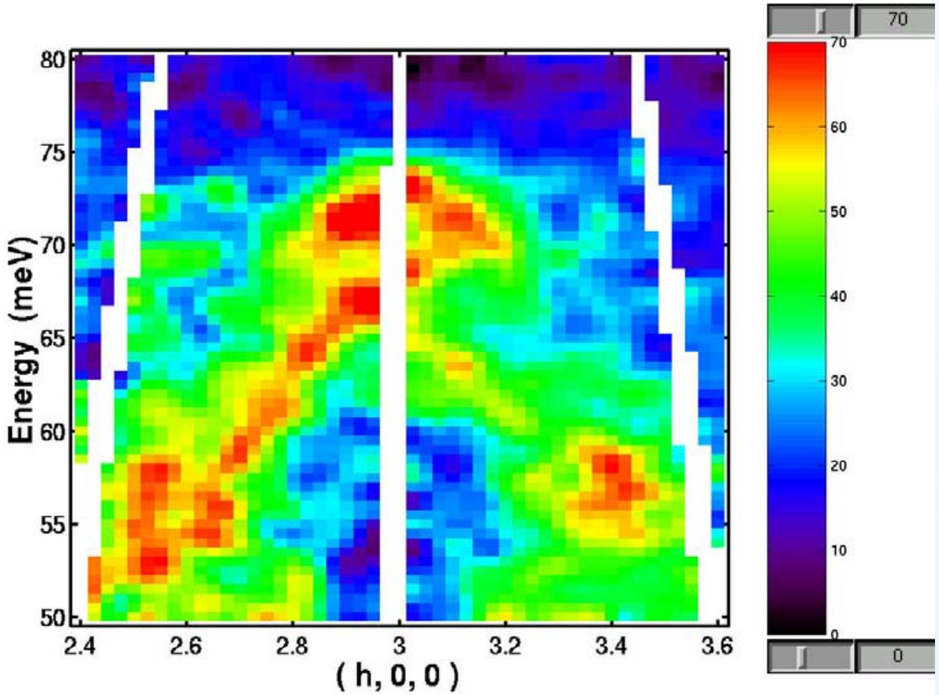


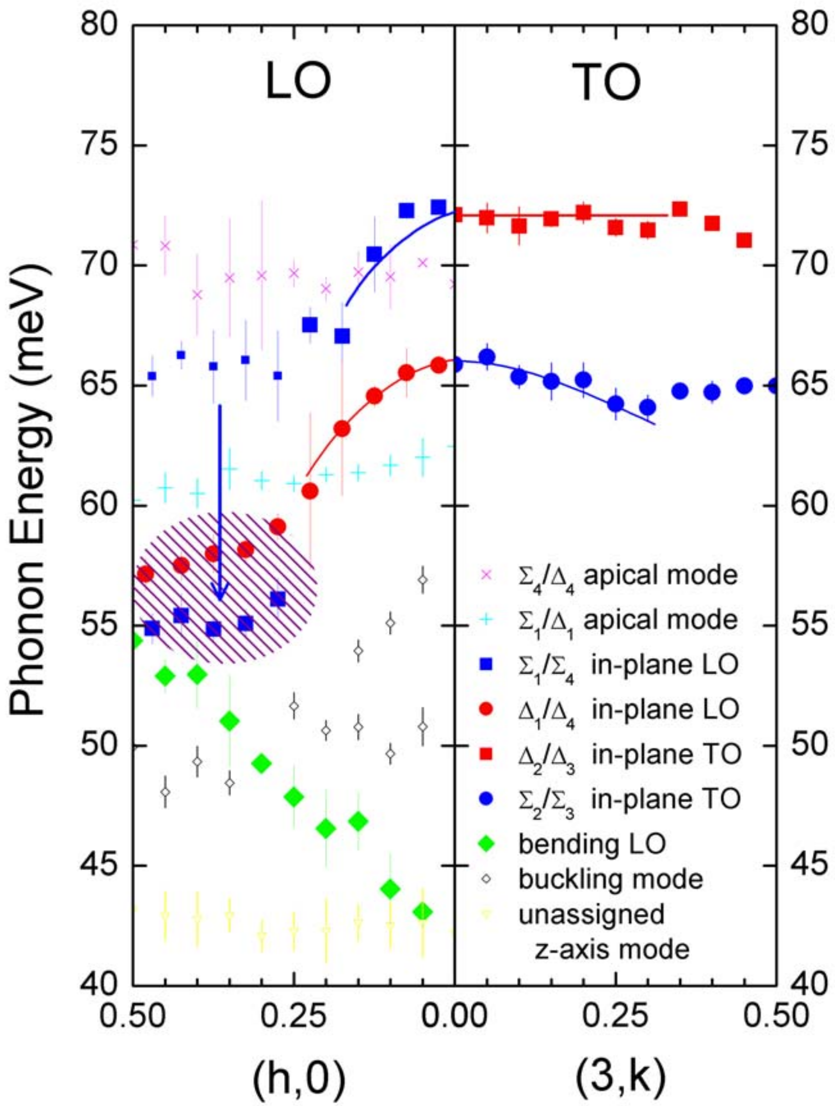
- Cu-O bond-stretching phonon mode induces strong charge transfer between Cu and O.

Born effective charge $Z^* = Z + \Delta Z \frac{a}{u}$

P. Piekarz and T. Egami, Phys. Rev. B **72**, 054530 (2005)

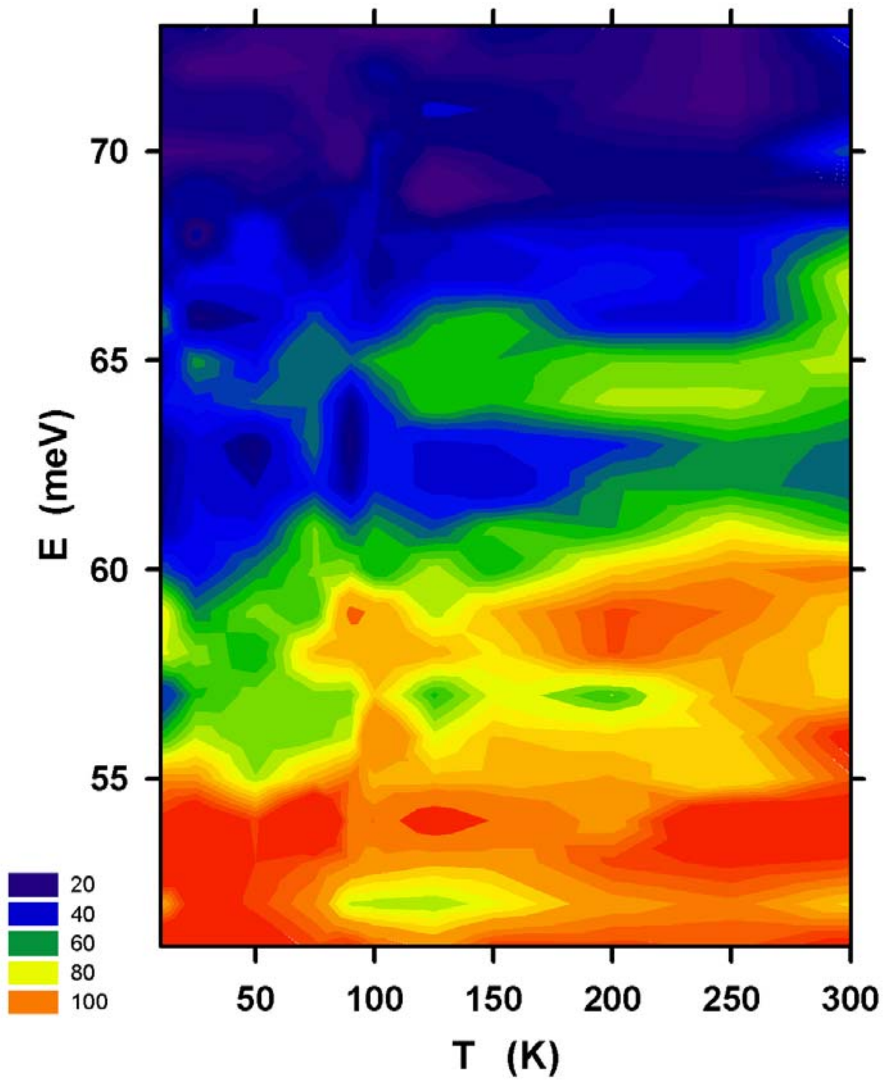
Cu-O Bond-stretching Mode, T = 110K





J.-H. Chung, et al, *Phys. Rev. B* 67, 014517 (2003)

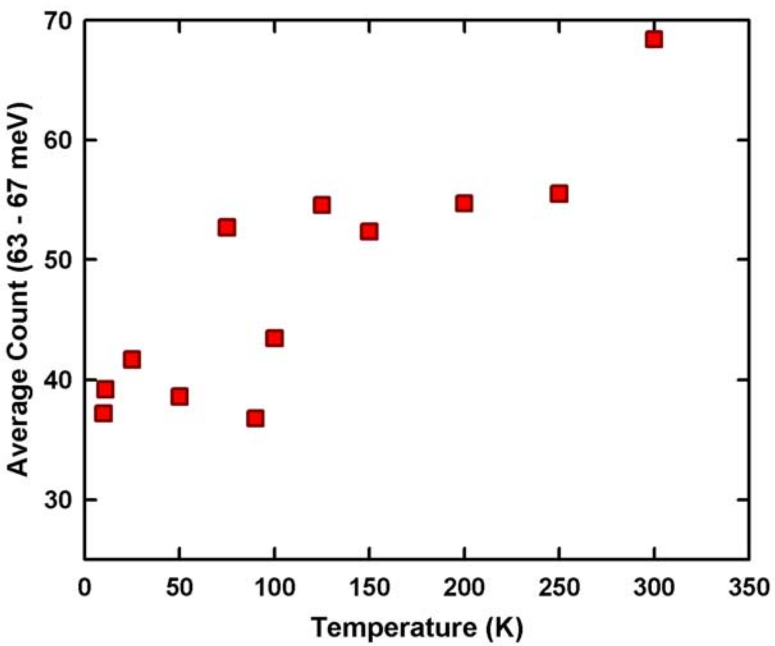
$YBa_2Cu_3O_{6.95}$ corrected for BE factor

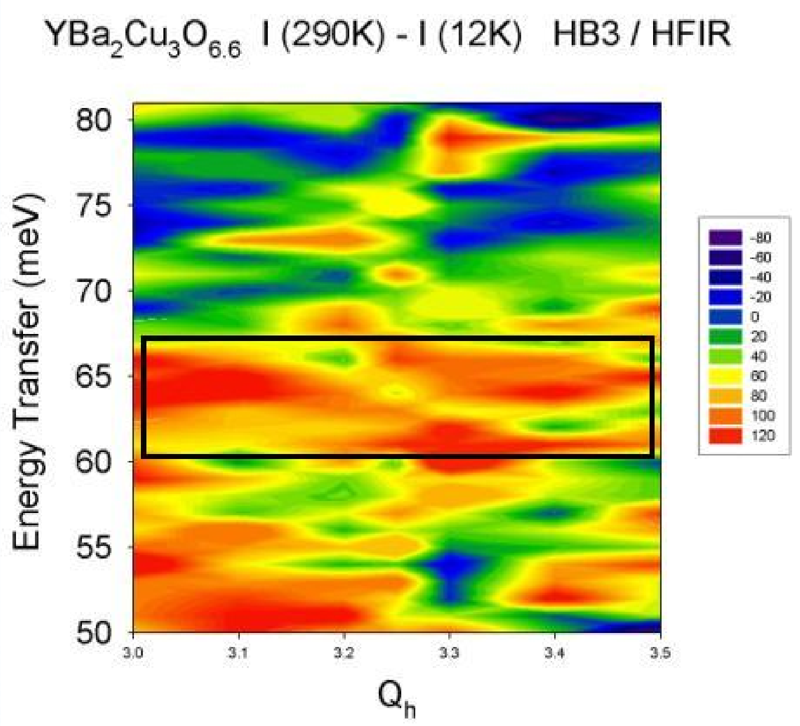


Temperature scan at (3.25, 0)

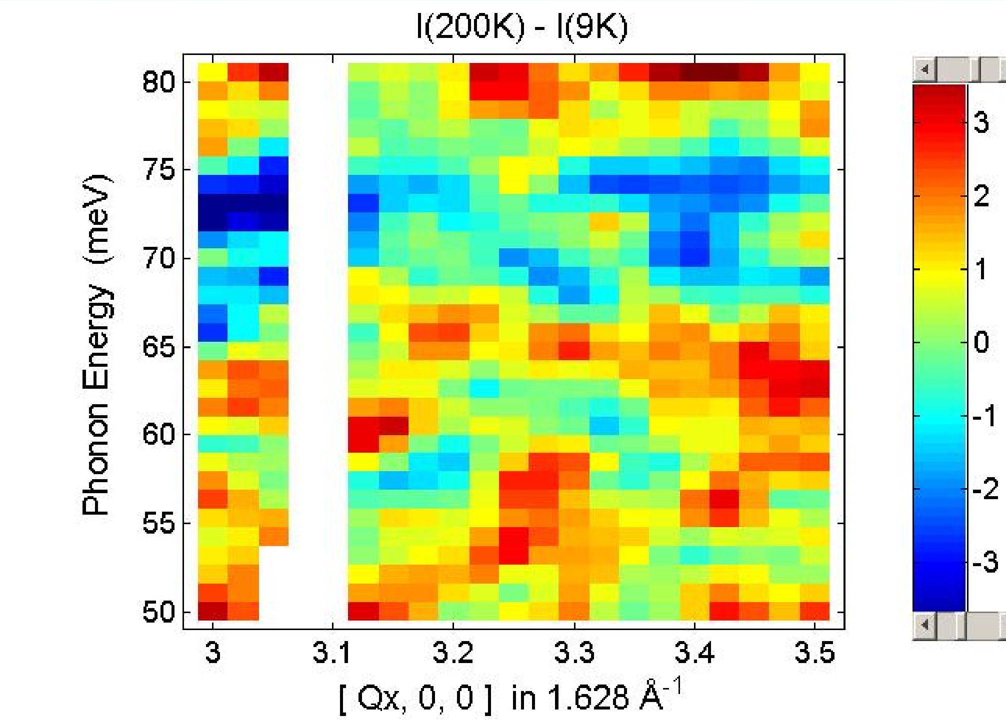
- The mode at 64 meV disappears below T_C (= 93 K).
- It softens to 53 meV below T_C.

I(63 – 67 meV)





HFIR data

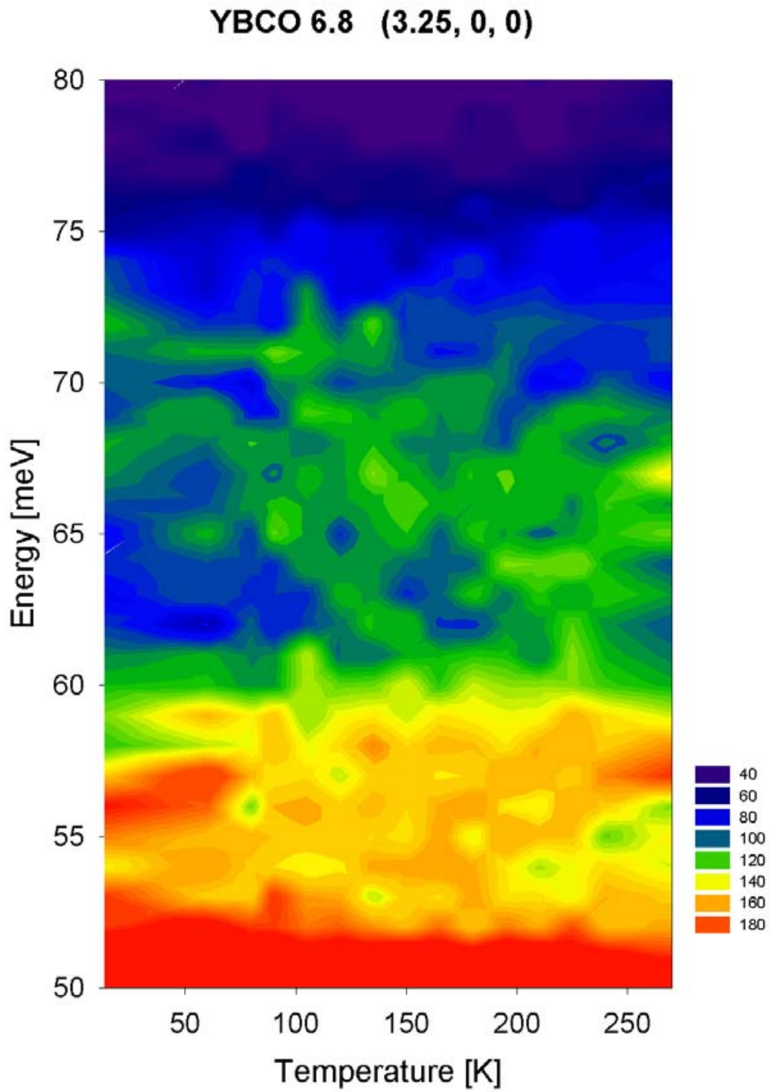


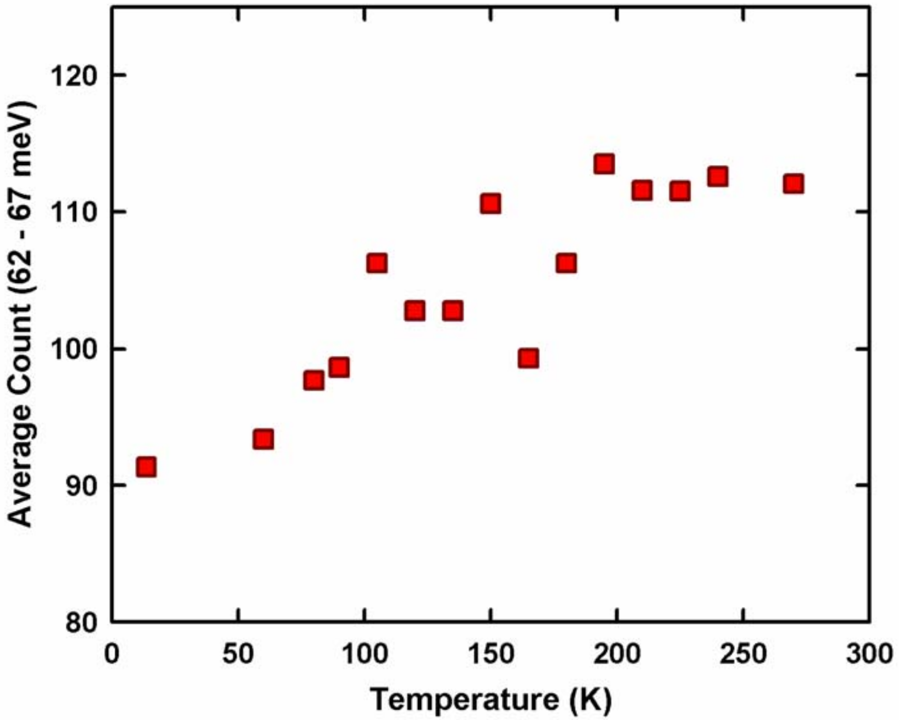
MAPS data

- A dispersionless (localized) mode at 64 meV at high temperatures. **The weight is about ¼.**
- Below T_{PG} it becomes dispersed.

YBCO6.8 (T_C = 80K)

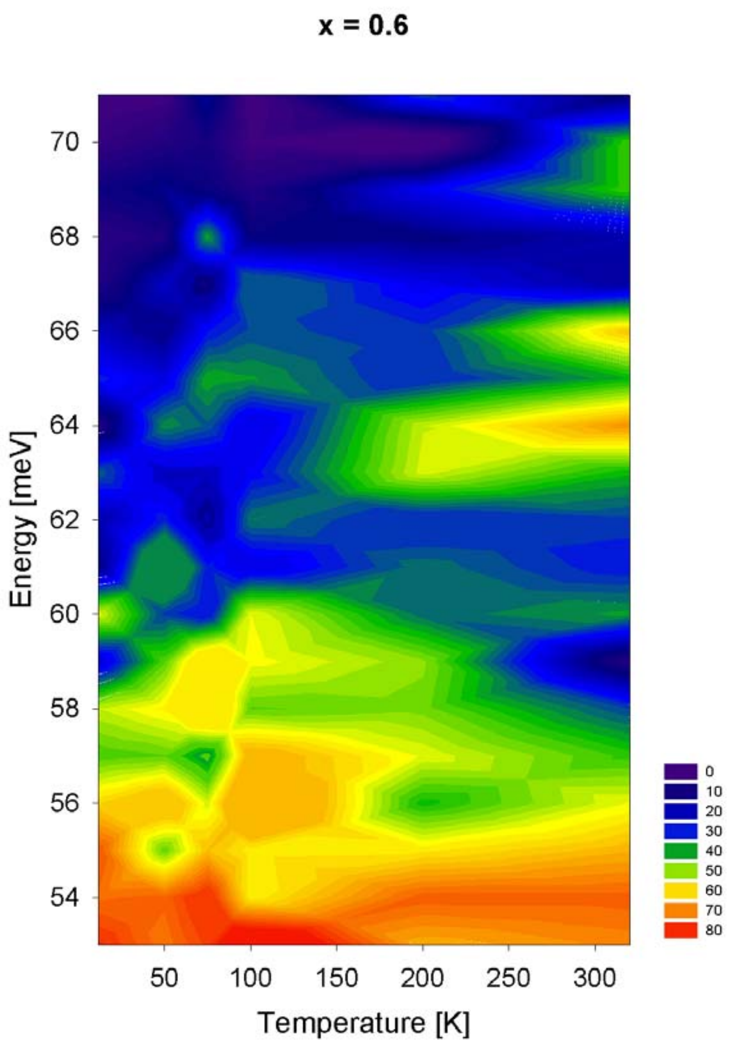
I(62 – 67 meV)

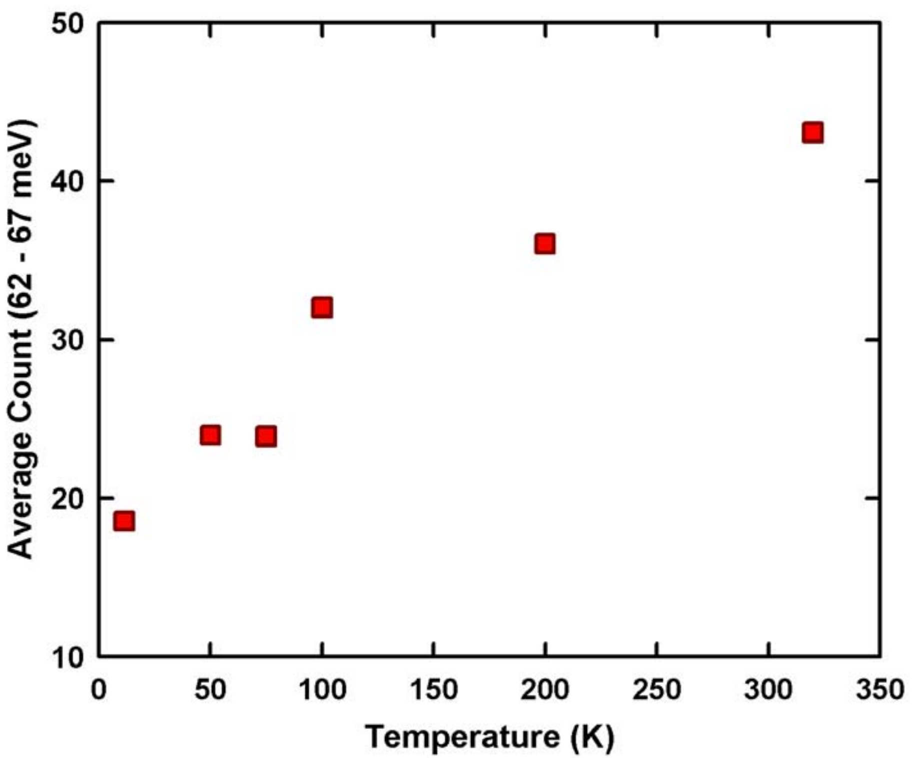




- For O(6.8) the extra mode, also around 64 meV, softens to 56 meV below T_{PG} (~160 K).

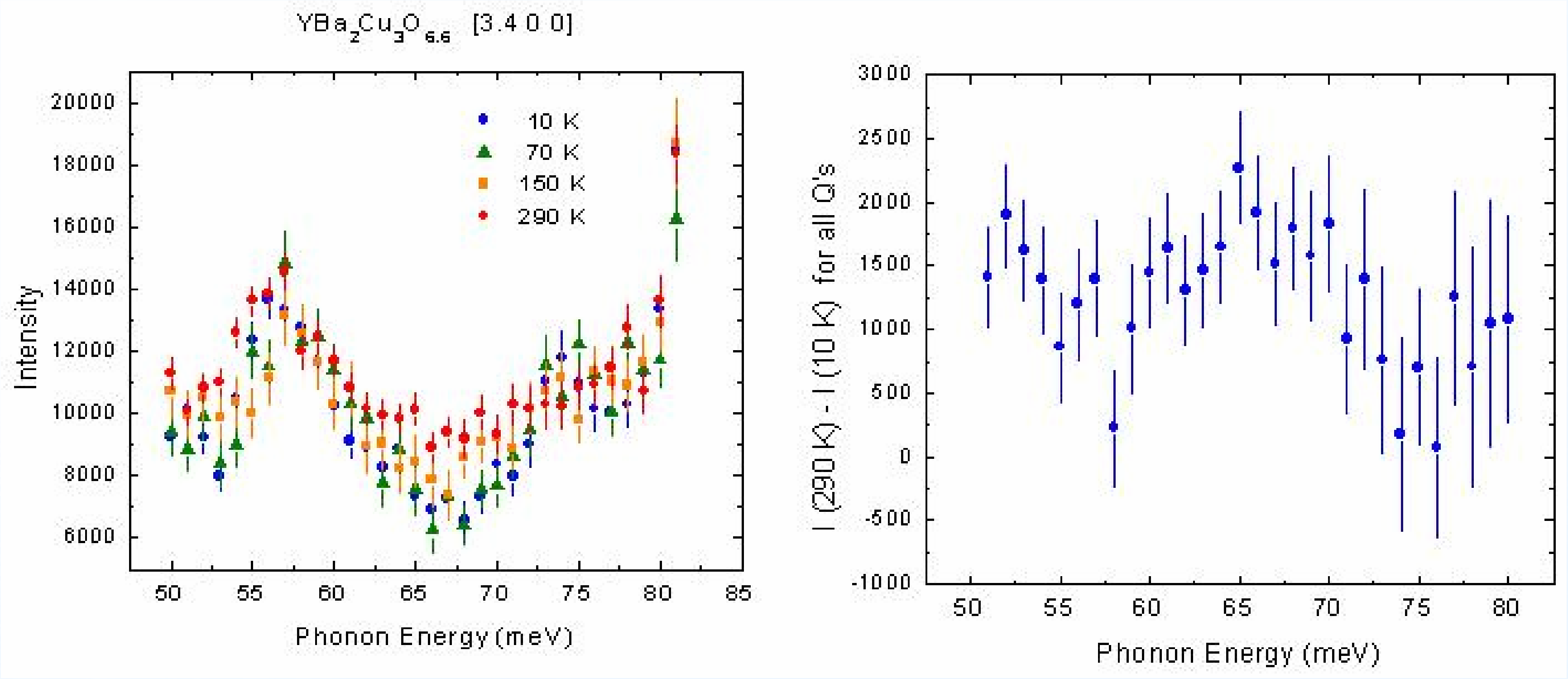
YBCO6.6 (T_C = 60K)





- 64 meV mode softens to 58 meV.

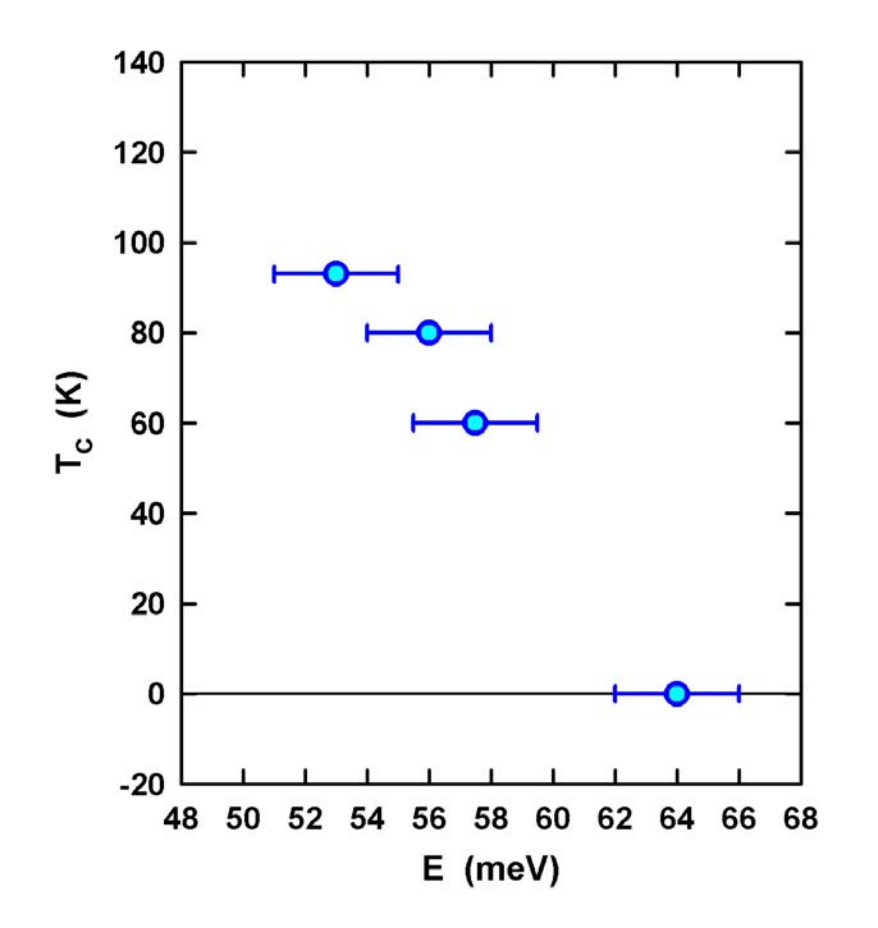
YBCO6.6 (T_C = 60 K)

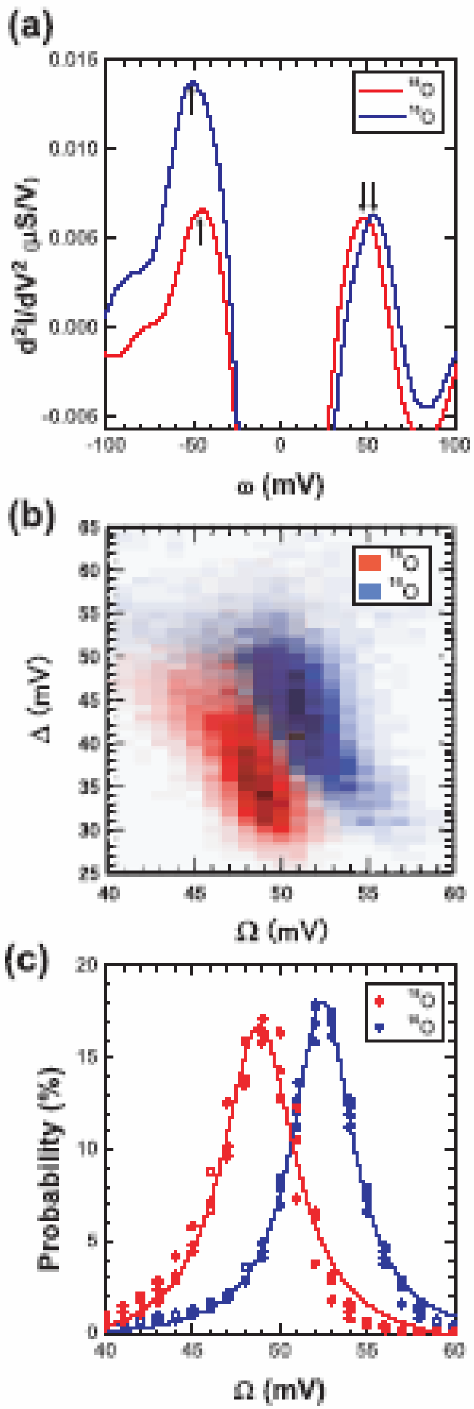


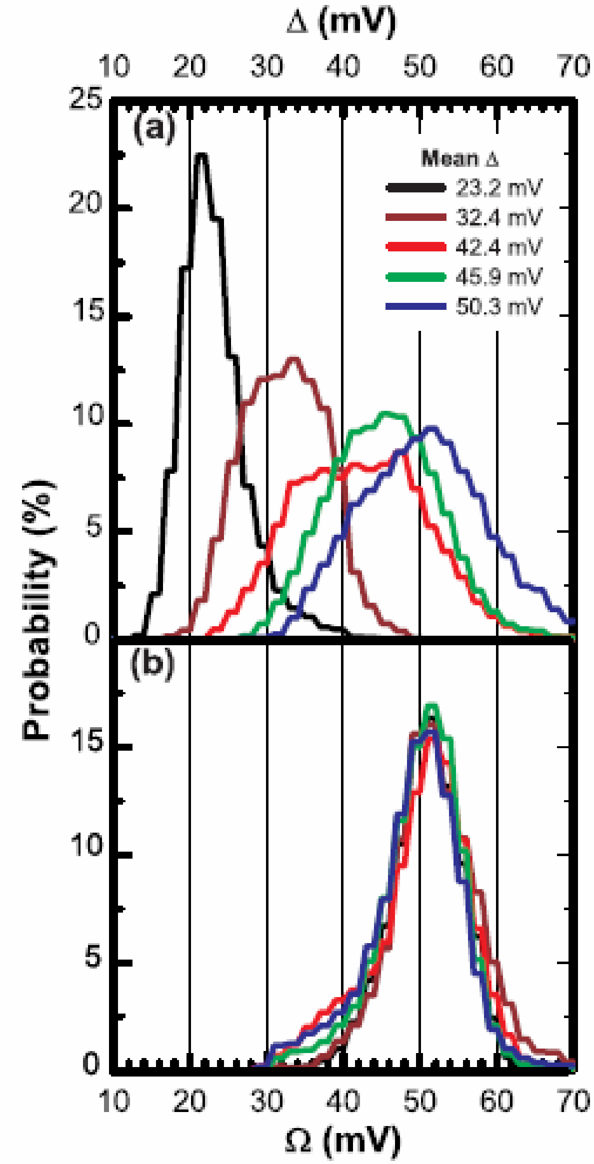
- Again the mode at 65 meV softens to 57.5 meV and 75 meV.

Phonon Softening

- Phonon softening linearly related to T_C (Uemura plot?).
- The amount (20 %) is anomalously large.







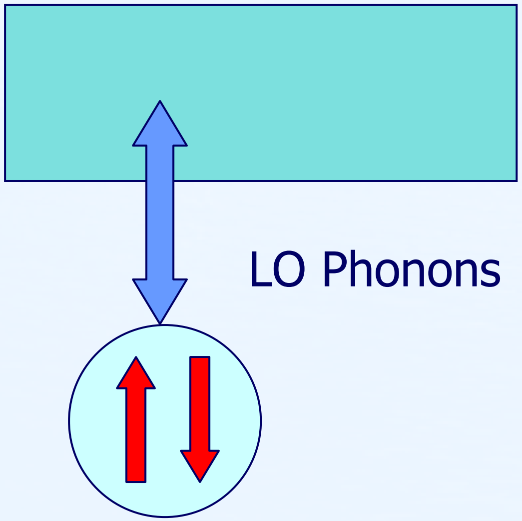
[Jinho Lee *et al Nature*, **442,** 546 (2006)]

Local Phonons and the Intermediate State

- The stripe state does not produce local states.
- The weight of the localized phonons is ¼.
- The intermediate state has the superlattice of at least 4 CuO_2 unit cells.
- Above T_{PG} the local structure must be random, leading to localization
- Below T_{PG} the long range order is restored.

Two-Component Model

- The localized object could be polarons (volume fraction ¼, around the anti-nodal point). Randomly distributed at HT.
- They may even be spin-singlet bipolarons.
- Two-components; localized bipolarons (bosons) and delocalized nodal fermions (Ranninger, Micnas, Bussmann-Holder).
- Interaction via the nodal fermions produces the intermediate order.
- Mediation by LO phonons is a possibility.



Conclusions

- The cuprates have the tendency of nano-scale phase separation into SC and non-SC (magnetic?) phases.
- The neutron scattering suggests that the origin of the pseudo-gap state may be magnetic.
- A peak observed by neutron scattering suggests a new intermediate phase, different from the stripe phase, may be formed.
- Intermediate state could hold the key in HTSC mechanism.