Electronic nematic susceptibility of iron-based superconductors

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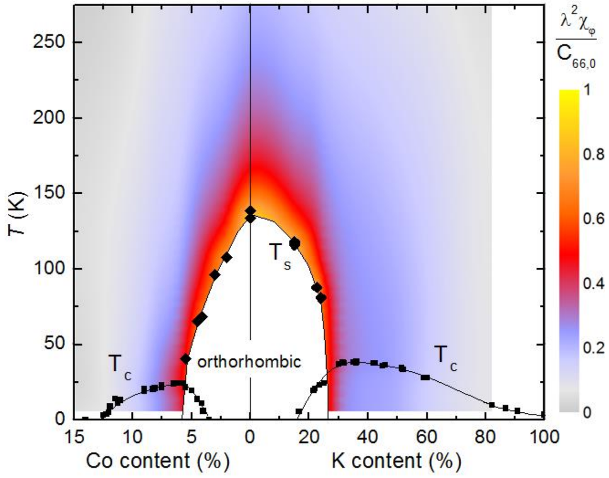
Institut für Festkörperphysik



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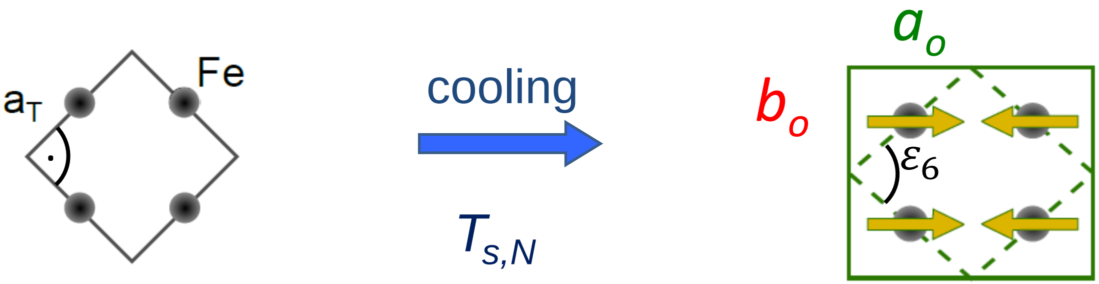
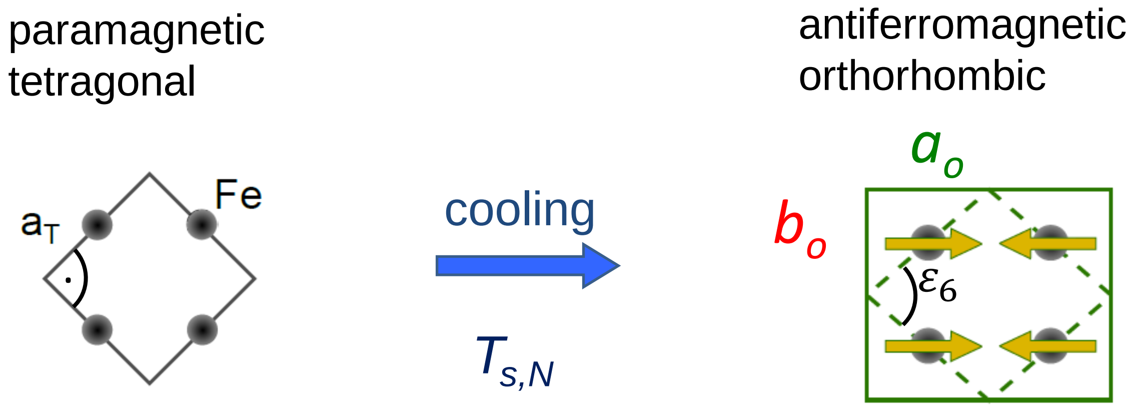
Stripe-type antiferromagnetism and orthorhombic distortion

paramagnetic
tetragonal

antiferromagnetic
orthorhombic



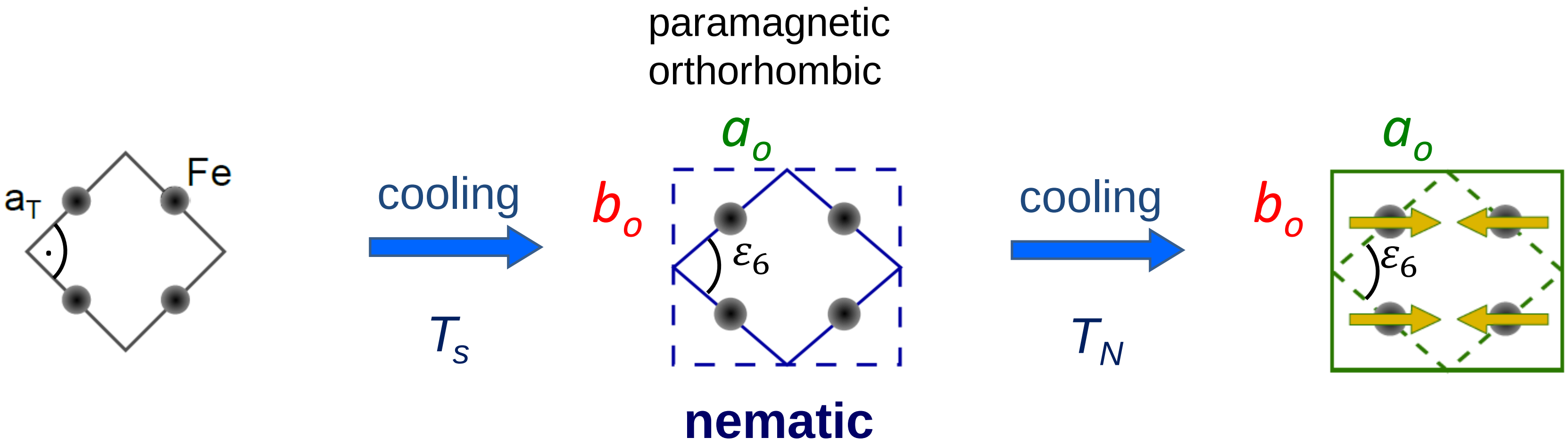
Stripe-type antiferromagnetism and orthorhombic distortion


paramagnetic
tetragonal

cooling

$T_{s,N}$

antiferromagnetic
orthorhombic


cooling

T_s

paramagnetic
orthorhombic

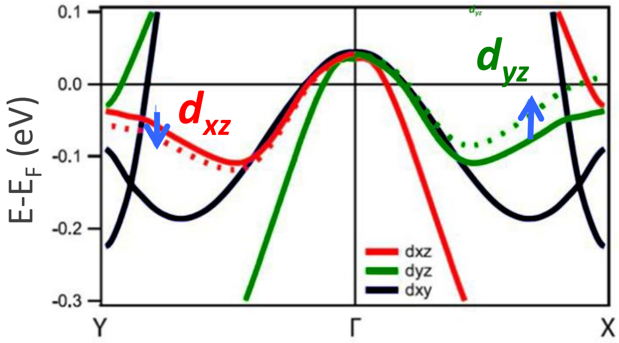
nematic

cooling

T_N

Two “pictures” for nematic order

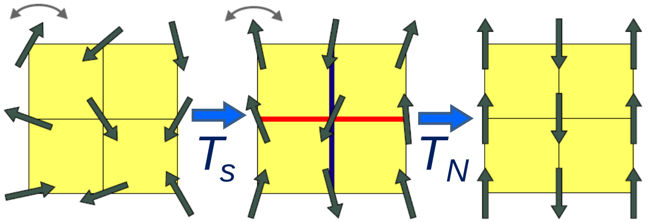
orbital picture:



- nematic order is orbital anisotropy (d_{xz} vs. d_{yz})
- magnetism is a secondary effect
- orbital fluctuations may mediate s++ superconductivity

Kontani et al. PRB. 2011

spin-nematic picture:



- magnetism is crucial
- nematic order is anisotropy of magnetic fluctuations
- spin fluctuations may mediate s+- superconductivity

Fernandes et al., Superconduct. Sci. Technol. 2012

Review: R. M. Fernandes et al., *What drives the nematic order in iron-based superconductors?* Nature Physics (2014)

Study both shear modulus and magnetic fluctuations (NMR)

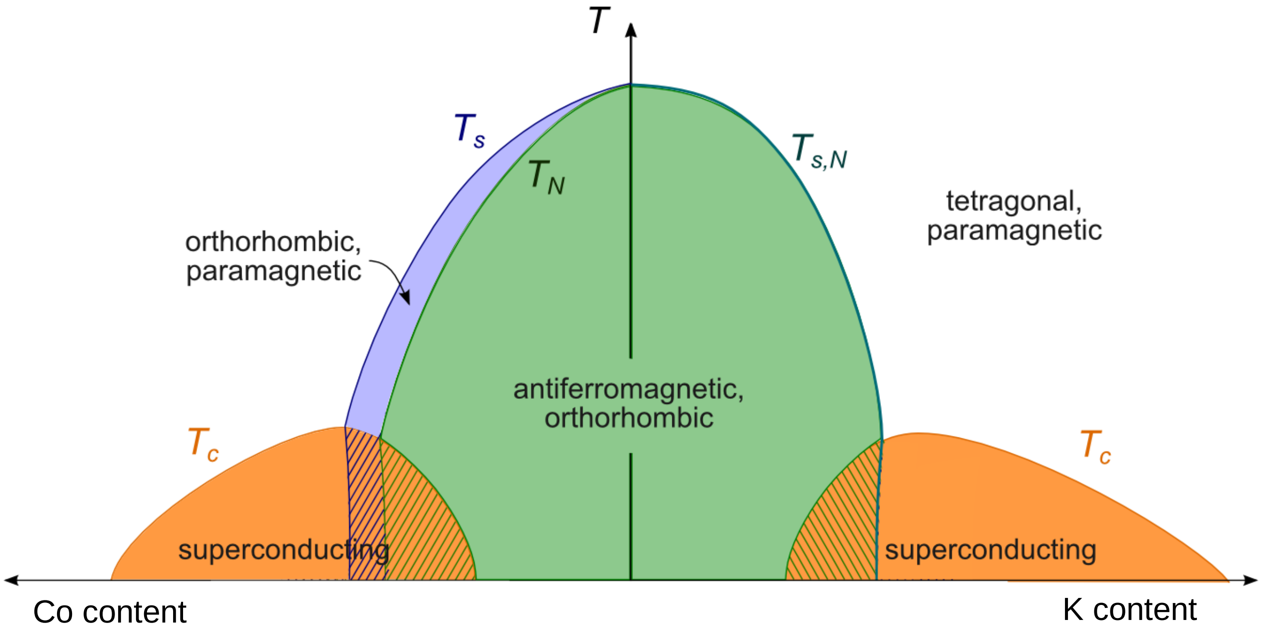
Three types of iron-based materials

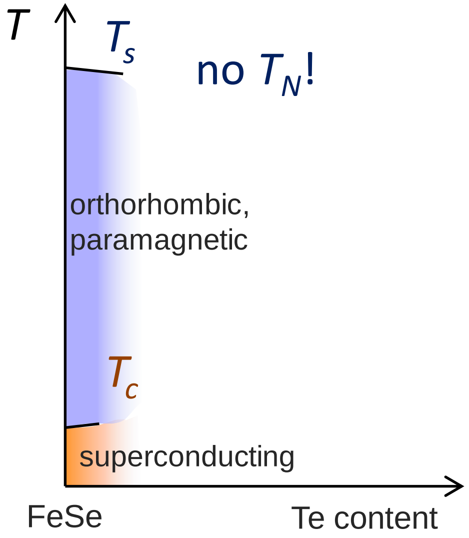
$BaFe_2As_2$

FeSe

$Ba(Fe,Co)_2As_2$
electron doped

$(Ba,K)Fe_2As_2$
hole doped

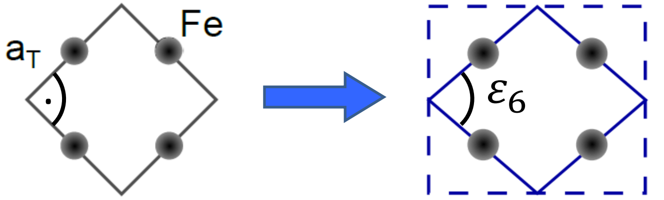




Outline

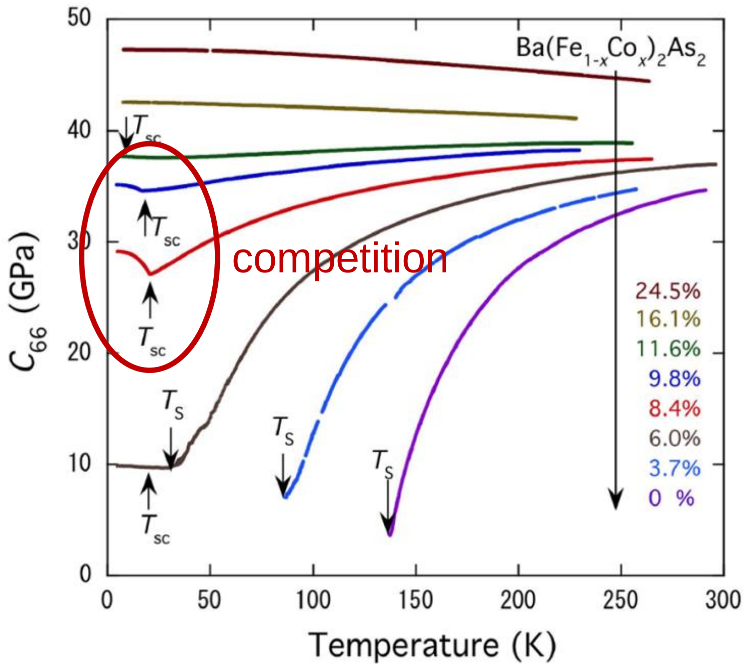
- Shear modulus, measured with a capacitance dilatometer
- Nematic susceptibility of electron- and hole-doped $BaFe_2As_2$
- Magnetic fluctuations at the origin of the structural transition?
- The case of FeSe: nematicity without magnetism?
- Conclusions

Doping dependence of C_{66} in $Ba(Fe,Co)_2As_2$ (ultrasound)

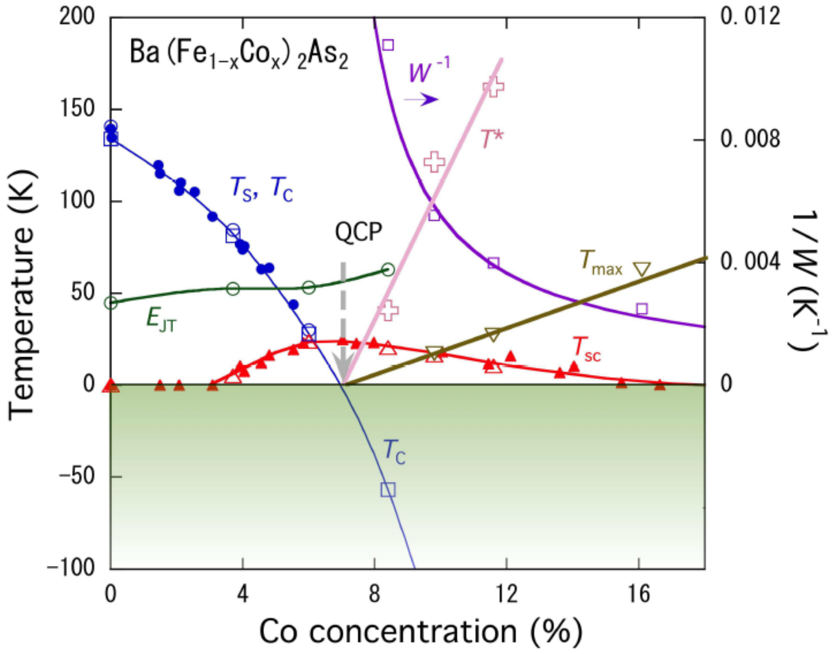


$$\sigma_6 = C_{66}\varepsilon_6$$

$$\varepsilon_6 = 1/C_{66}\ \sigma_6$$



competition



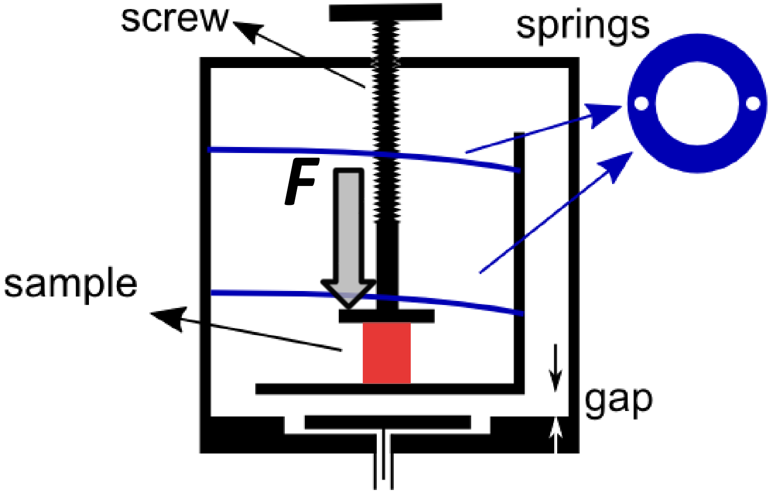
Yoshizawa et al. JPSJ 2012
also: Fernandes et al. PRL 2010
Goto et al. JPSJ 2011

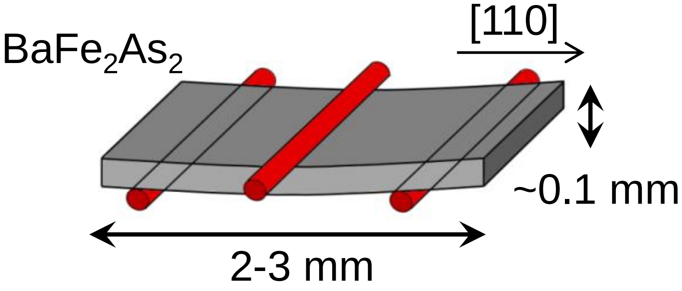
What about the other systems?

Alternative way to measure elastic constants – using a capacitance dilatometer

Three-point bending!

resolution: 0.1-0.01 Å





“New” method: thin crystals are ideal, don‘t need to be perfect

Alternative way to measure elastic constants – using a capacitance dilatometer

Three-point bending!

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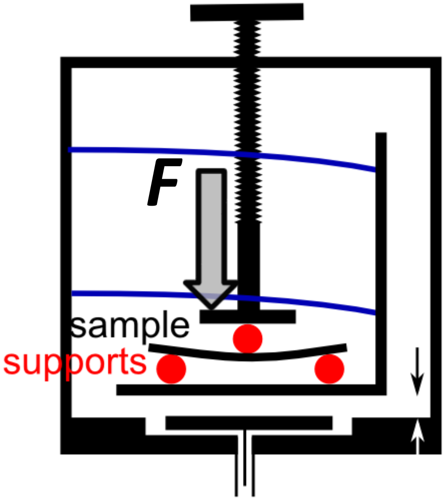
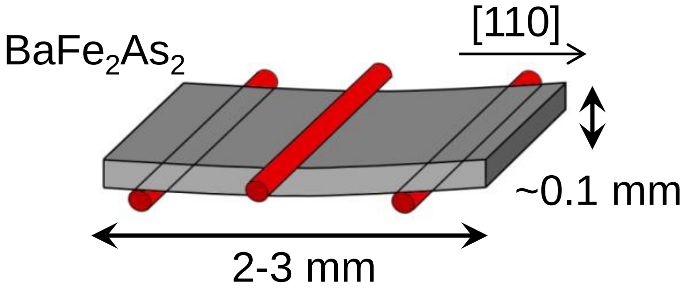
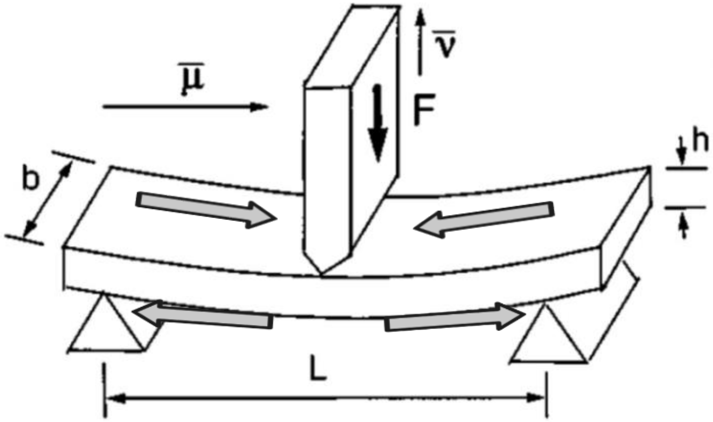


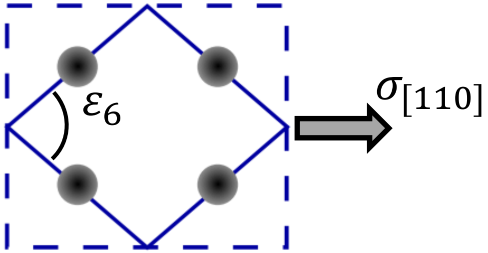


“New” method: thin crystals are ideal, don‘t need to be perfect

What is measured in three-point bending?



Young‘s modulus: $Y_{\vec{\mu}} = \sigma_{\vec{\mu}}/\varepsilon_{\vec{\mu}}$



$$k \approx 4b\left(\frac{h}{L}\right)^3 Y_{[110]}$$

$$\propto 4\left(\frac{1}{C_{66}}+\frac{1}{\gamma}\right)^{-1} \text{with}$$

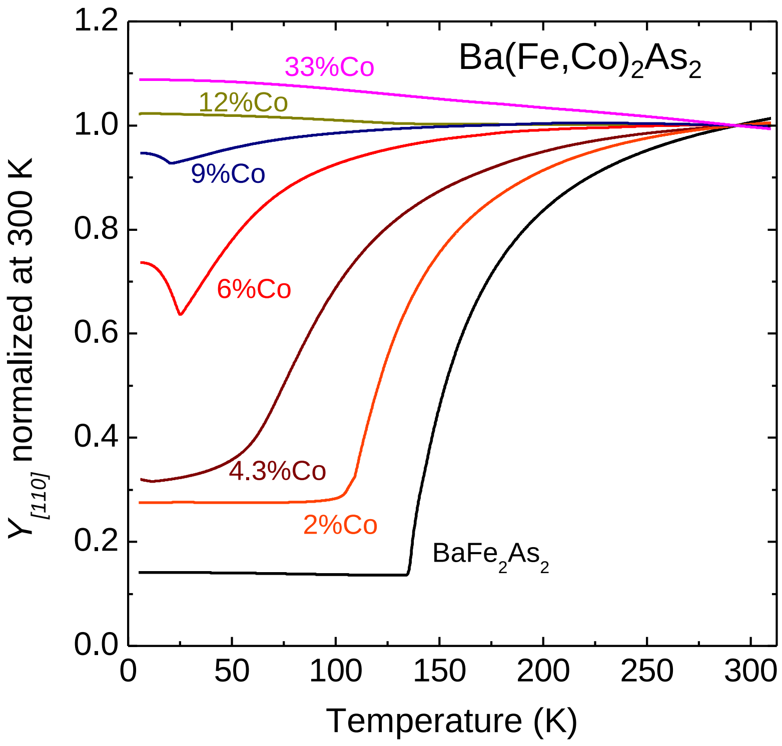
$$\gamma = \frac{C_{11}}{2}+\frac{C_{12}}{2}+\frac{C_{13}^2}{C_{33}}$$

See Kityk et al., PRB 2000

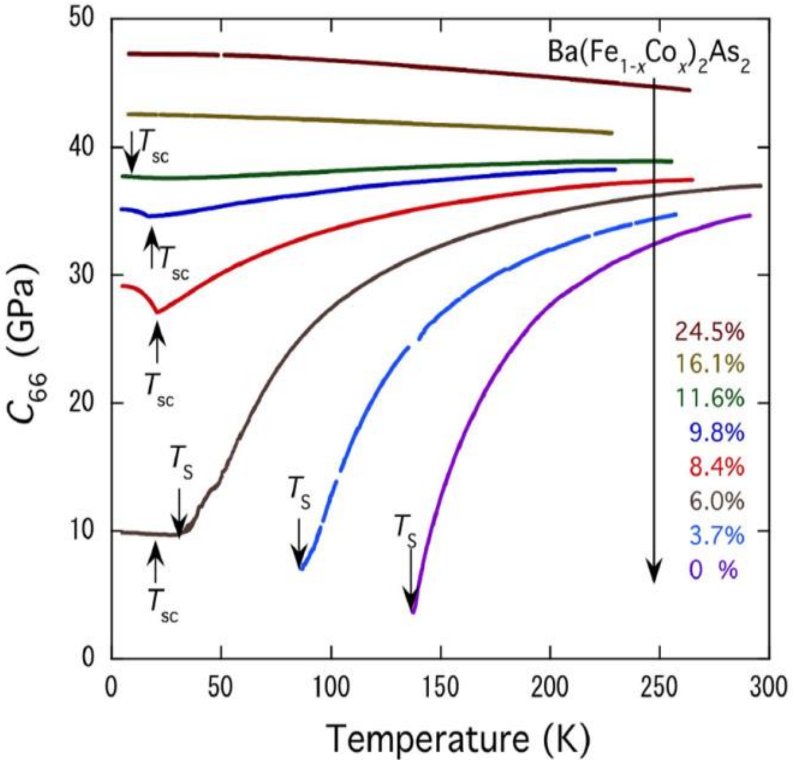
$Ba(Fe,Co)_2As_2$: Comparison with literature data

$$Y_{[110]} = 4\left(\frac{1}{C_{66}} + \frac{1}{\gamma}\right)^{-1} \text{with } \gamma = \frac{C_{11}}{2} + \frac{C_{12}}{2} + \frac{C_{13}^2}{C_{33}}$$

Young‘s modulus $Y_{[110]}$ with bending technique

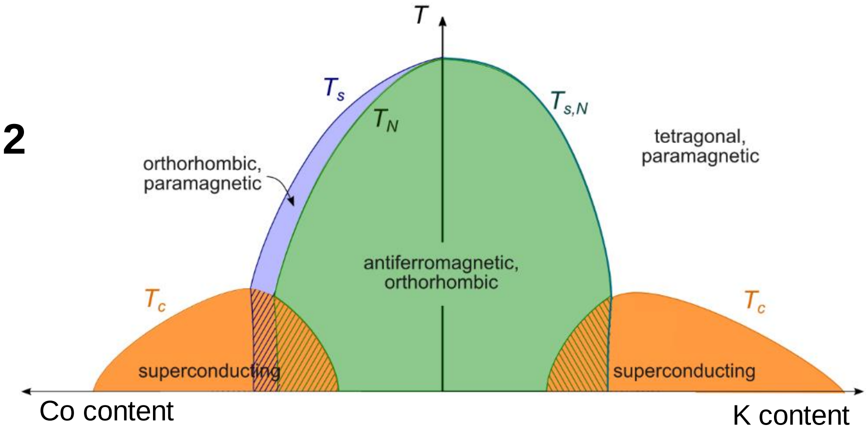


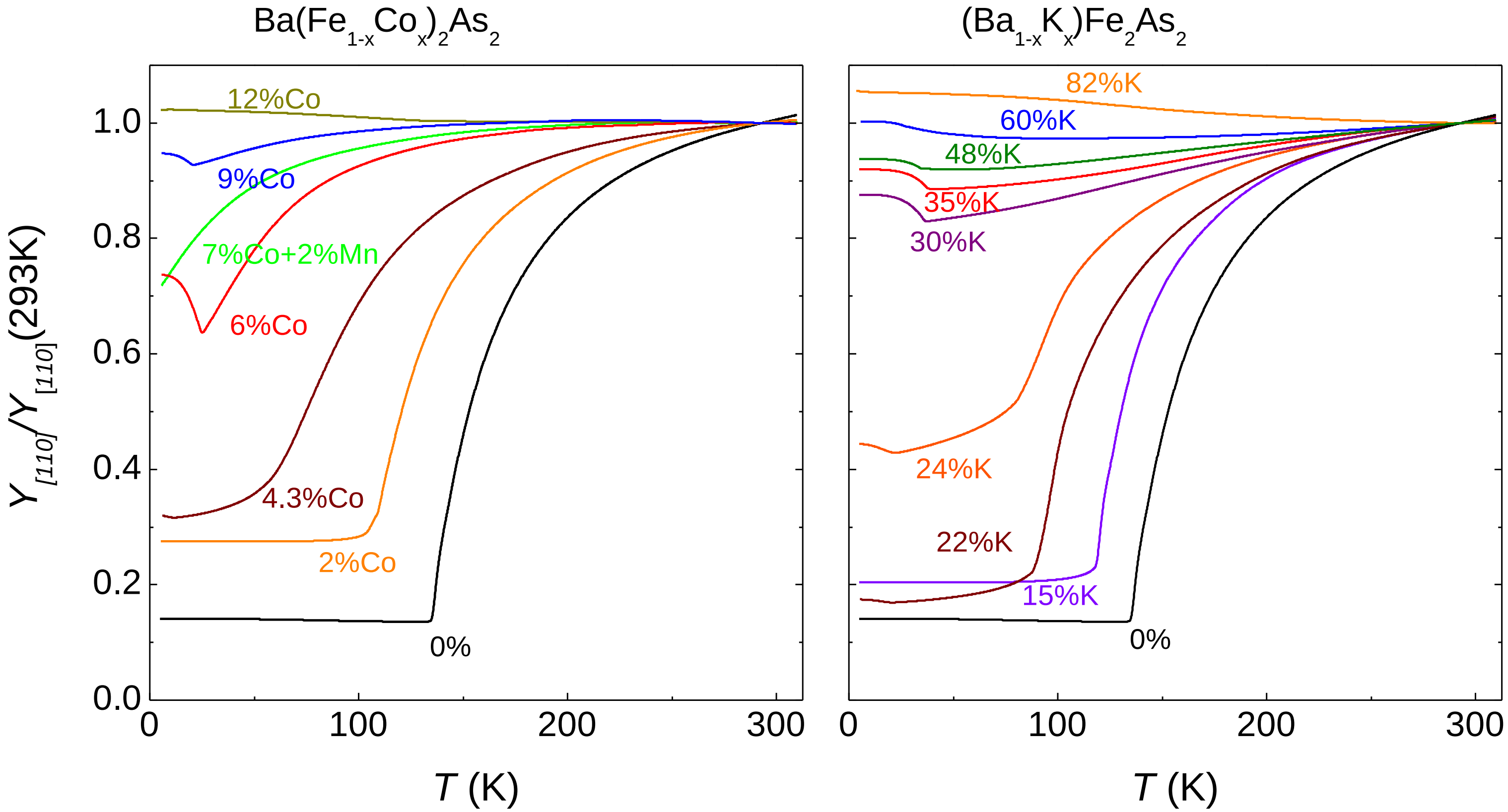
Shear modulus C_{66} from ultrasound



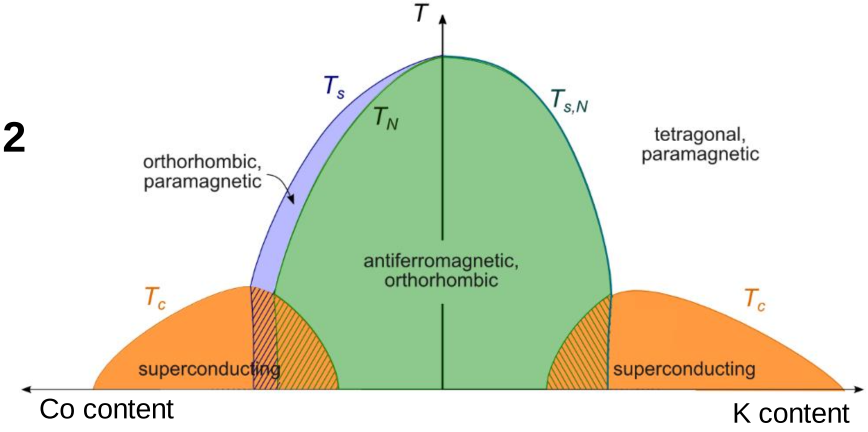
Yoshizawa et al., JPSJ 2012

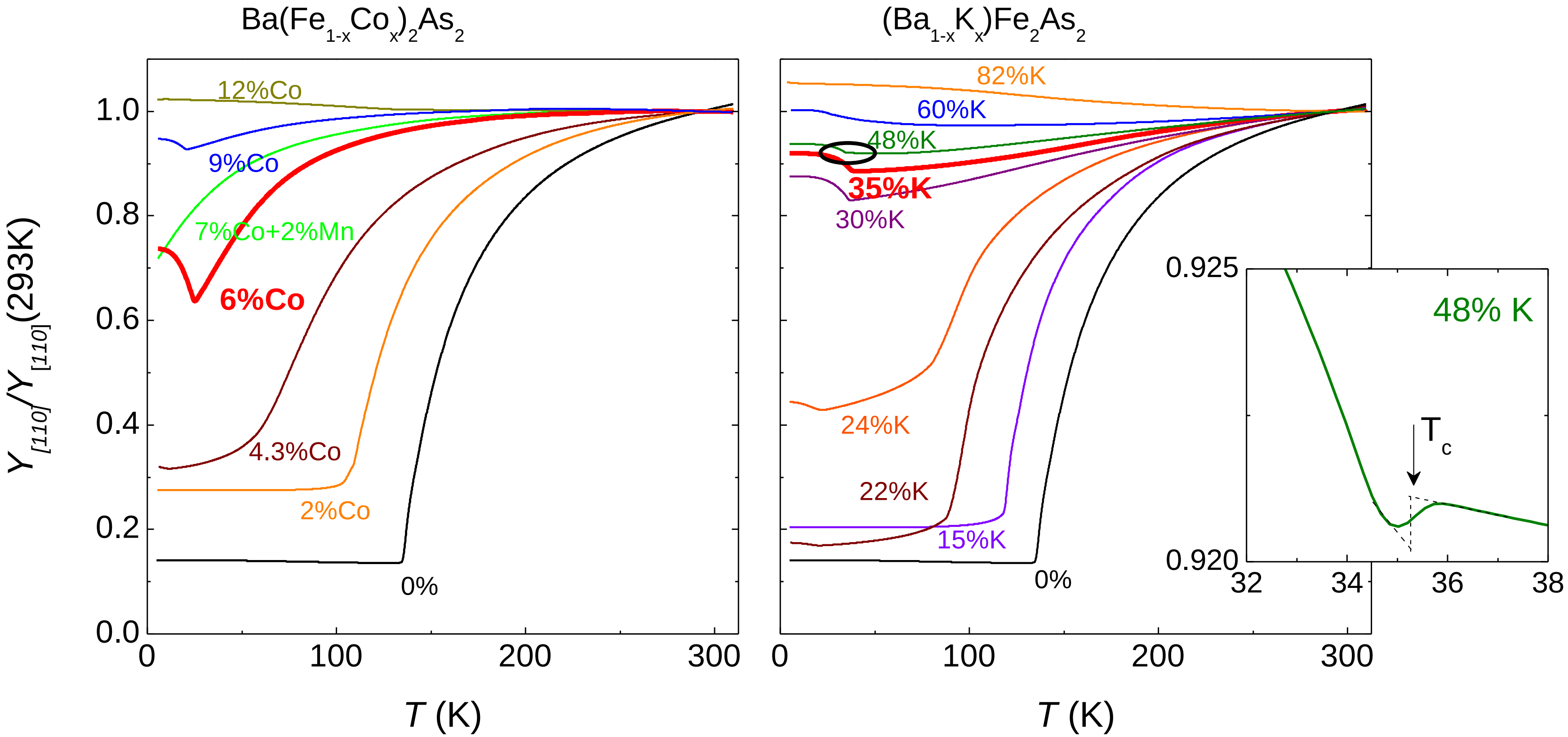
$Ba(Fe,Co)_2As_2$ vs. $(Ba,K)Fe_2As_2$





Ba(Fe,Co)$_2$As$_2$ vs. (Ba,K)Fe$_2$As$_2$





Nematic susceptibility from the shear modulus

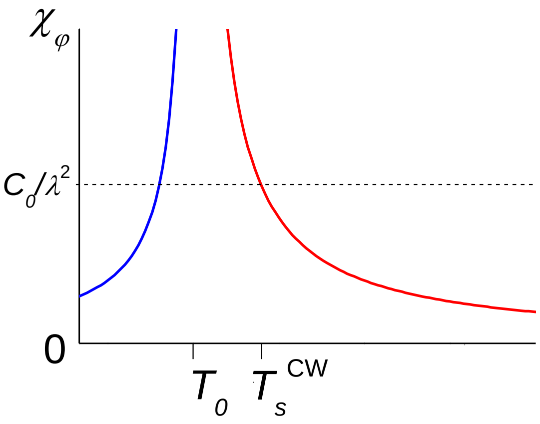
Free energy

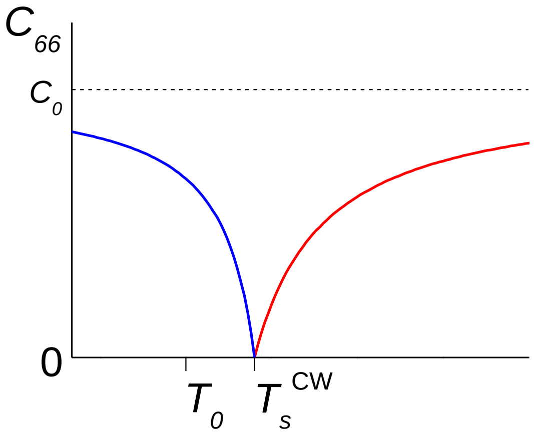
$$F(\varepsilon_6, \varphi) = \frac{C_{66,0}}{2}{\varepsilon_6}^2 - \lambda\varepsilon_6\varphi + \frac{1}{2}\left(\chi_\varphi\right)^{-1}\varphi^2 + \frac{B}{4}\varphi^4$$

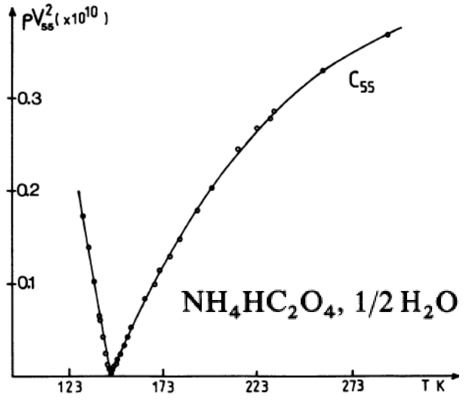
ε_6, orthorhombic distortion
λ, electron-lattice coupling constant
φ, nematic order parameter (symmetry!)
χ_φ, nematic susceptibility (at $\varepsilon_6 = \text{constant}$, or $\lambda = 0$)

Shear modulus

$$\frac{d^2F}{d\varepsilon_6^2} = C_{66} = C_{66,0} - \lambda^2\chi_\varphi \quad (T > T_s)$$



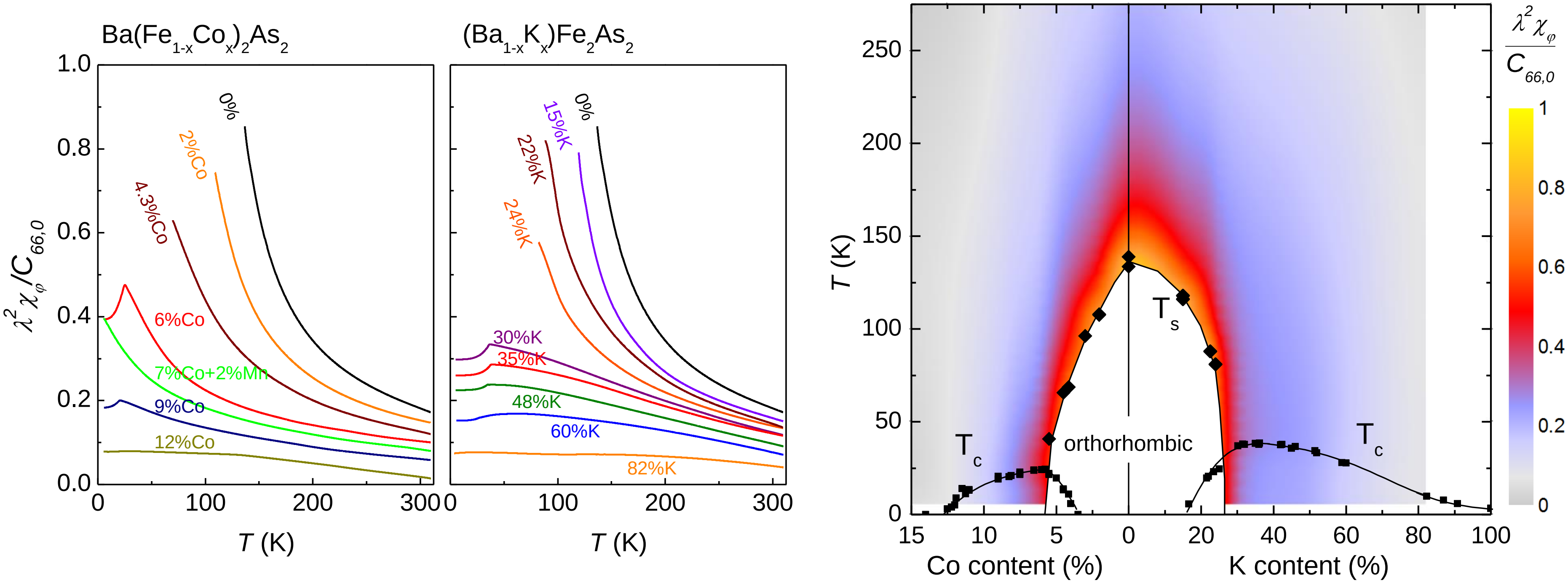




see e.g. Benoît et al., J. Physique 1986
Fernandes et al., PRL 2010
Chu et al., Science 2012

Nematic susceptibility of $Ba(Fe,Co)_2As_2$ and $(Ba,K)Fe_2As_2$

$$C_{66} = C_{66,0} - \lambda^2 \chi_\varphi$$



Phonon background $Y_0(T)$ is given by sample with 33% Co content

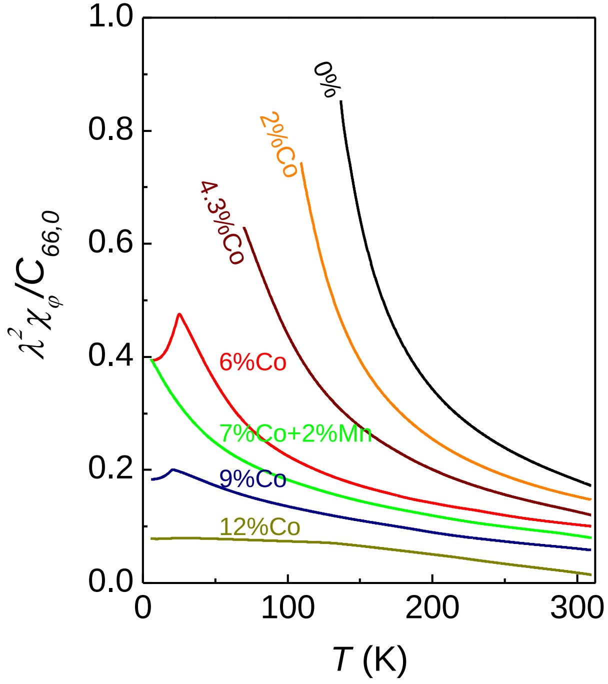
Approximation: $Y_{[110]}/Y_0 \approx C_{66}/C_{66,0} = 1 - \frac{\lambda^2\chi_\varphi}{C_{66,0}}$

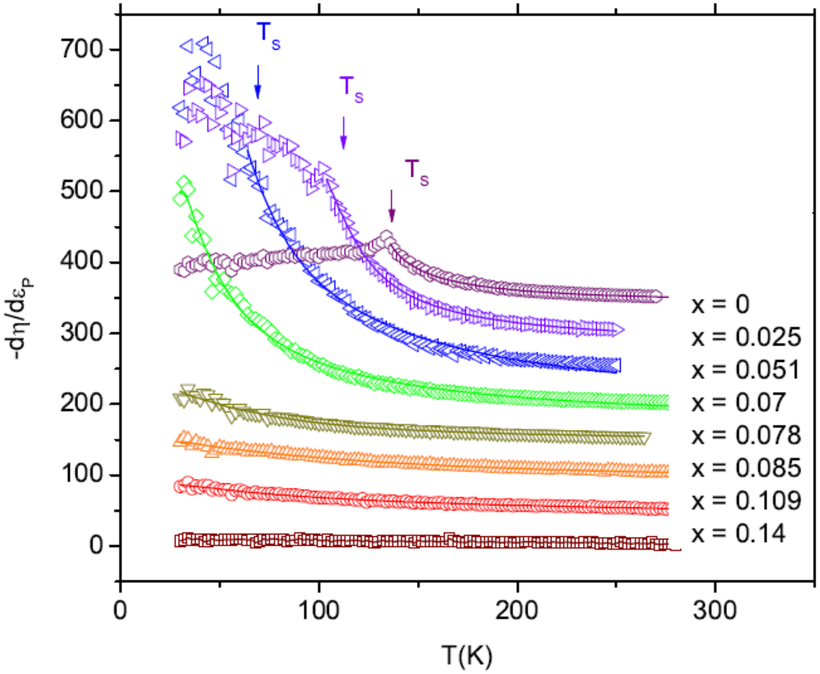
Comparison with strain derivative of resistivity anisotropy in $Ba(Fe,Co)_2As_2$

Chu et al. Science 2012

$$C_{66} = C_{66,0} - \lambda^2 \chi_\varphi$$

$$\frac{dN}{d\varepsilon_6} \propto \lambda \chi_\varphi$$



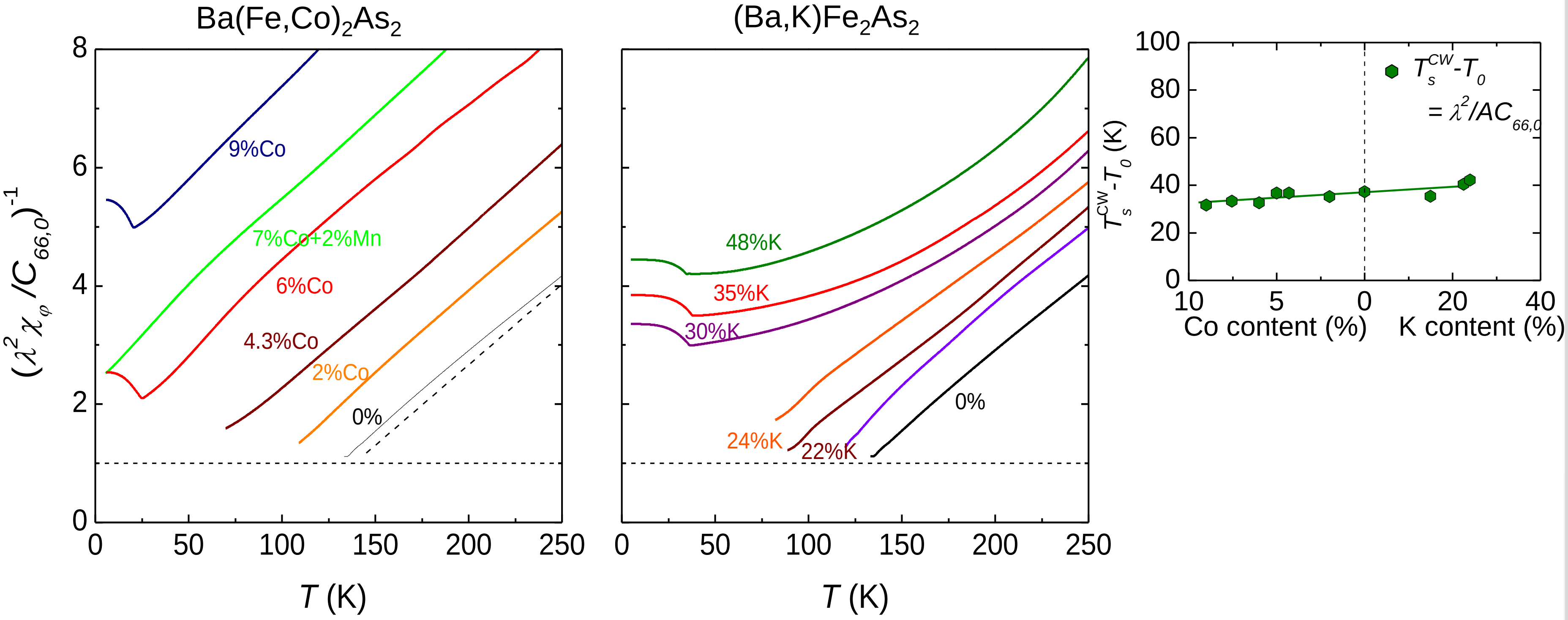


Temperature dependence of the nematic susceptibility

Curie-Weiss law:

$$\chi_\varphi(T) = \frac{1}{A(T - T_0)}$$

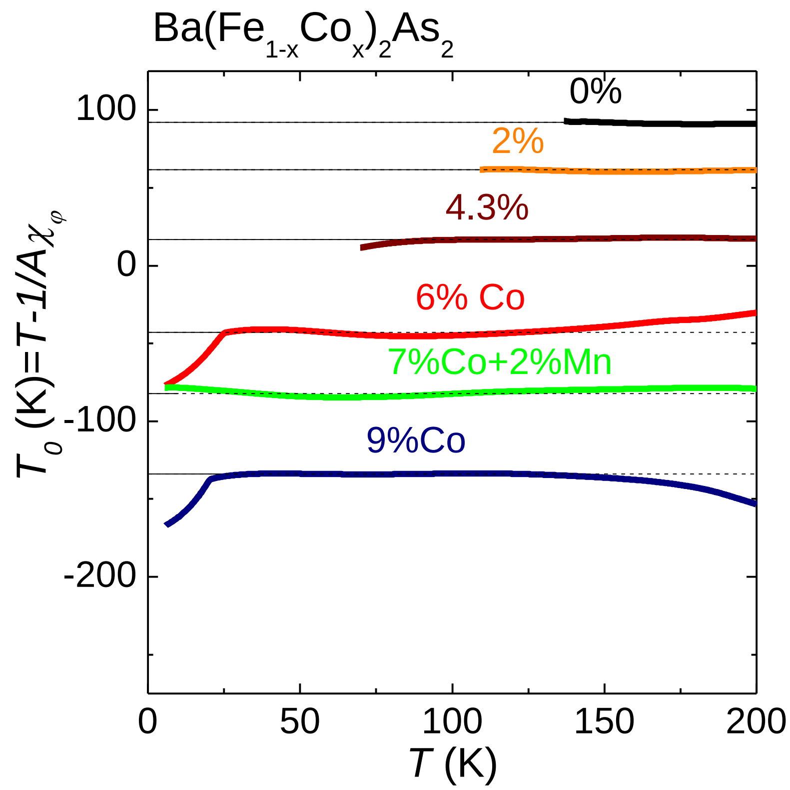
$$T_s^{\mathrm{CW}} = T_0 + \frac{\lambda^2}{AC_{66,0}}$$



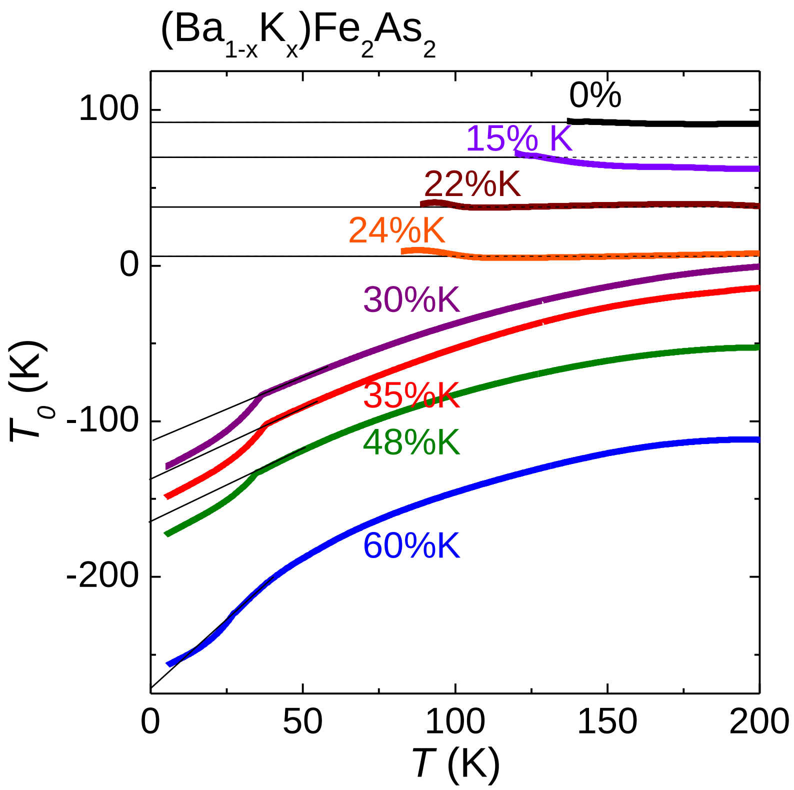
In what way is overdoped (Ba,K)Fe_2As_2 different?

- Parameterize deviations by a temperature dependent T_0

$$\chi_\varphi(T) = \frac{1}{A(T - T_0(T))}$$

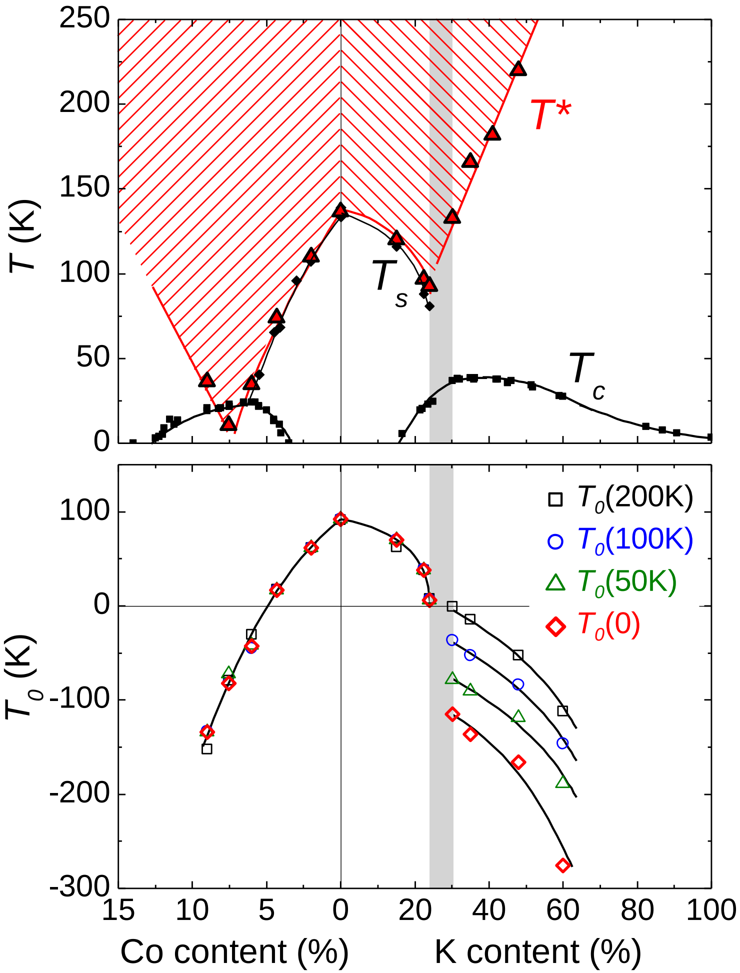


$Ba(Fe_{1-x}Co_x)_2As_2$



$(Ba_{1-x}K_x)Fe_2As_2$

Phase diagram from nematic susceptibility



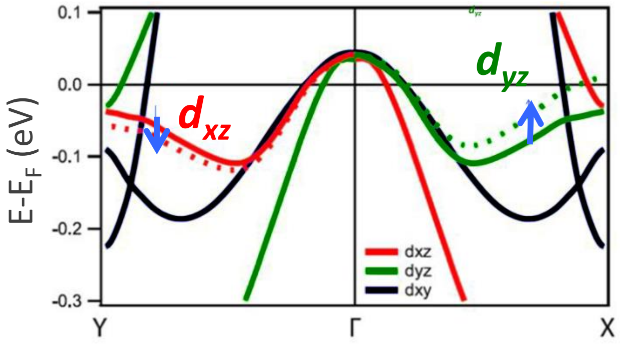
- No critical $\sim 1/(T - T_0)$ softening in optimally doped (Ba,K)Fe_2As_2
- Abrupt change of temperature dependence of the nematic susceptibility at 24%-30% K content

- Possible quantum critical point in Ba(Fe,Co)$_2As_2$
- QCP preempted by a first-order transition in (Ba,K)Fe_2As_2

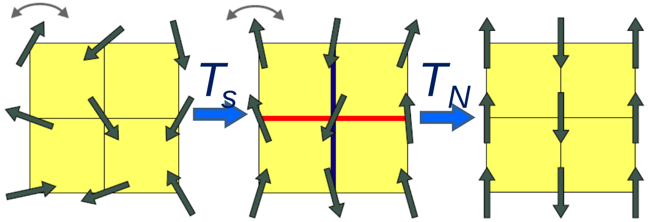
A. Böhmer et al., PRL 112, 047001 (2014)

How to distinguish between the two pictures

orbital picture:

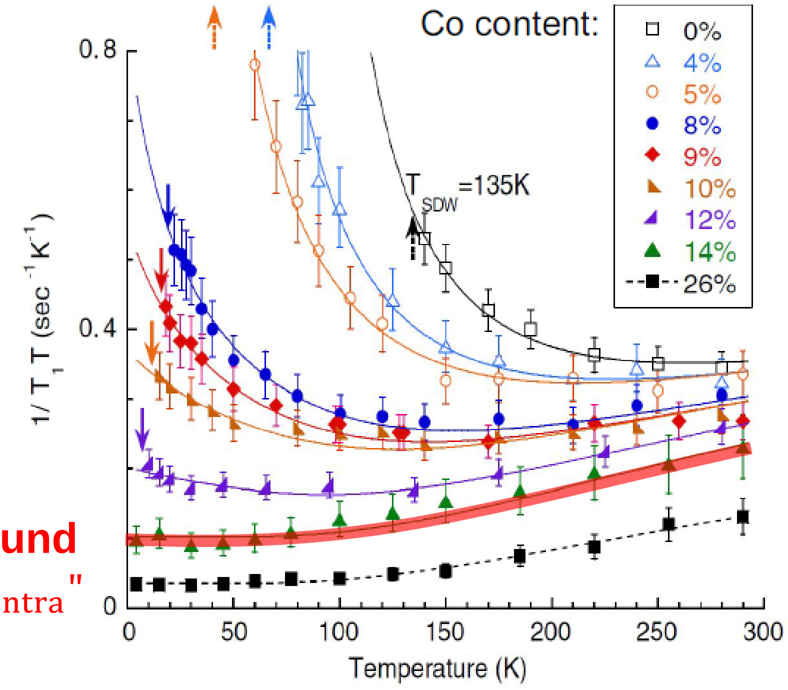


spin-nematic picture:



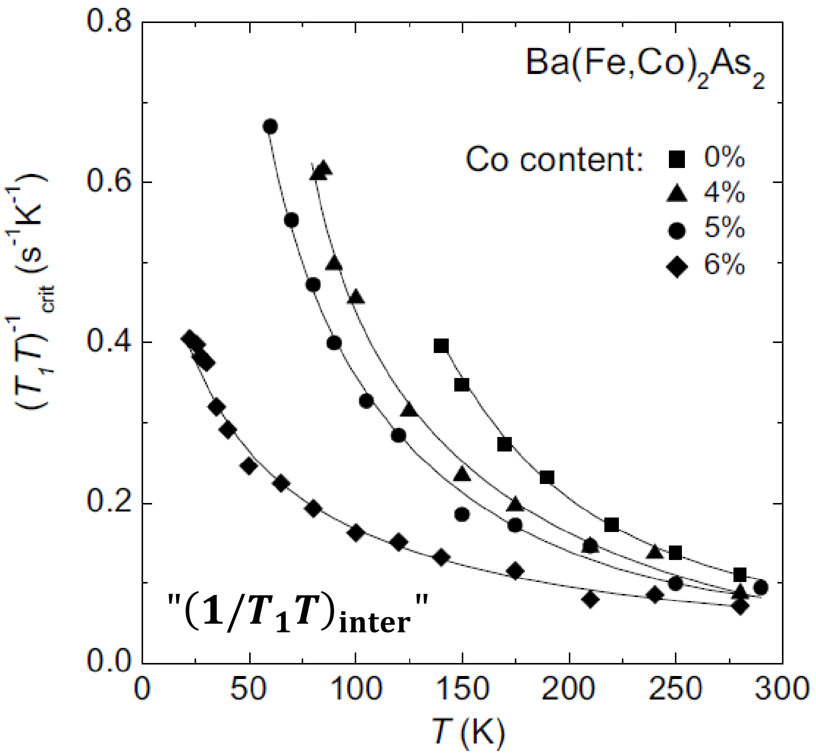
Study magnetic fluctuations (NMR)

The spin-lattice relaxation rate $1/T_1T$ in Ba(Fe,Co)$_2$As$_2$



background

"$(1/T_1T)_{\mathrm{intra}}$"



"$(1/T_1T)_{\mathrm{inter}}$"

$$(1/T_1T)_{\mathrm{intra}} = \alpha + \beta \exp(-\Delta/k_B T)$$

$$(1/T_1T)_{\mathrm{inter}} = C/(T + \theta)$$

Ning et al., PRL 2010

Shear modulus in the spin-nematic scenario

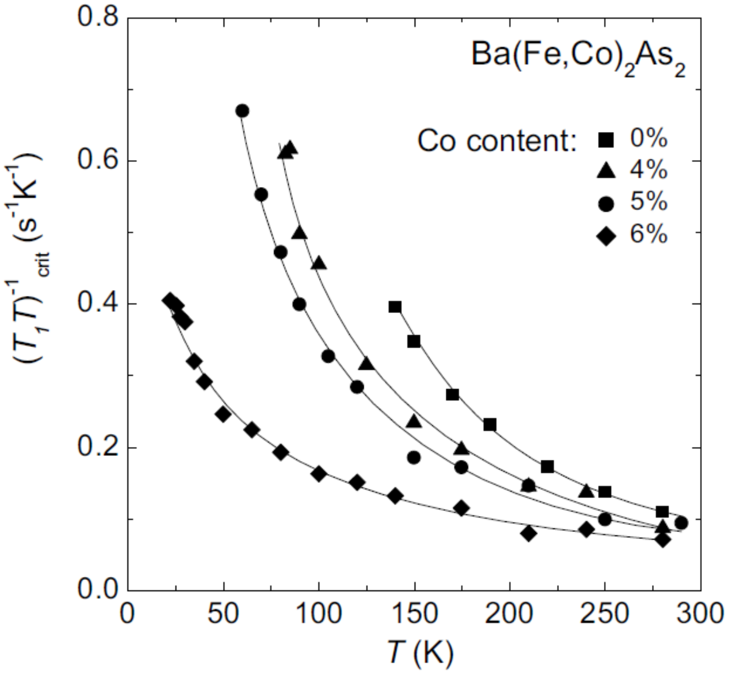
$$\chi_\varphi = \frac{\sum_q \chi^2(q)}{1 - g_0 \sum_q \chi^2(q)}$$

$$\frac{1}{T_1 T} = \gamma_g^2 \lim_{\omega \to 0} \sum_{\mathbf{k}} F^2(\mathbf{k}) \frac{\mathrm{Im}\, \chi(\mathbf{k}, \omega)}{\omega}$$

$$\sum_q \chi^2(q) \propto (T_1 T)^{-1}$$

$$C_{66} = C_{66,0} - \lambda^2 \chi_\varphi$$

$$\frac{C_{66}}{C_{66,0}} = \frac{1}{1 + [a(T_1 T) - b]^{-1}}$$

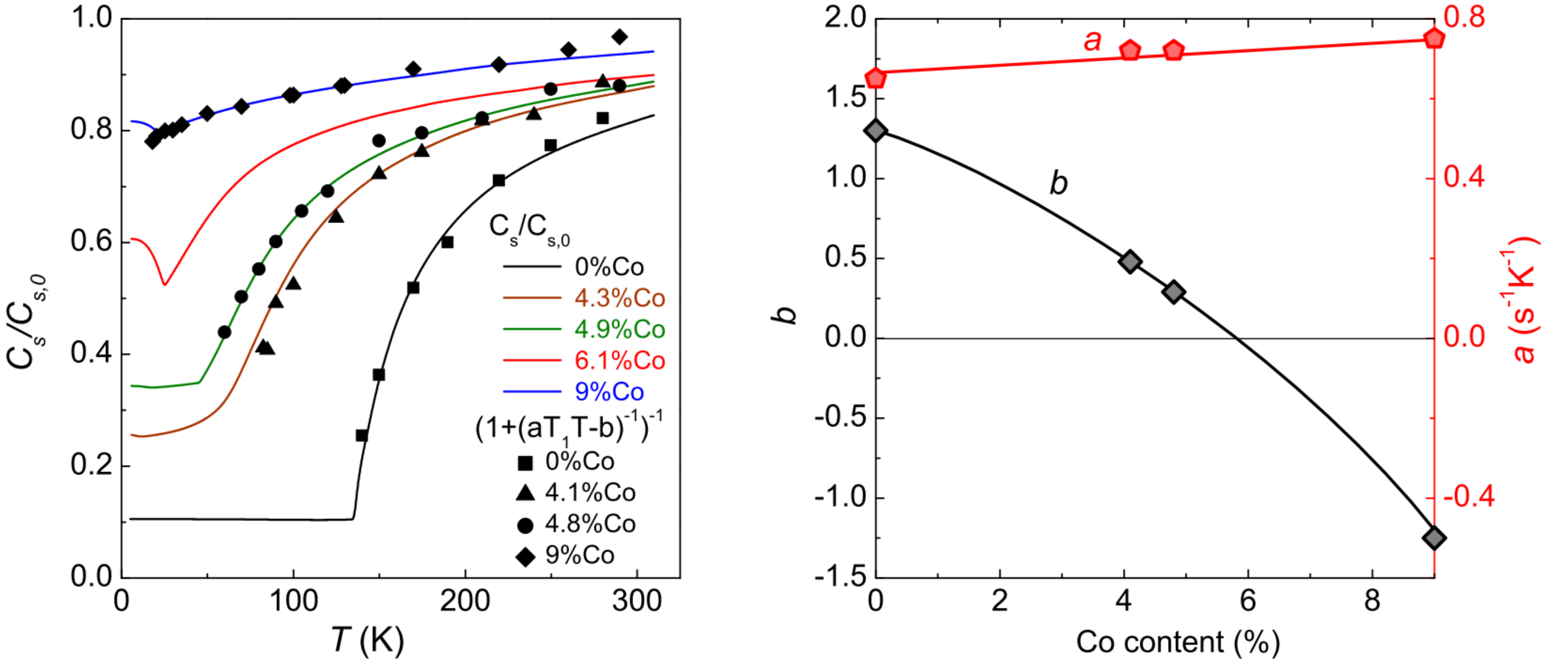


Spin-lattice relaxation time T_1 should scale with shear modulus

R. M. Fernandes et al., PRL 111, 137001 (2013)

Scaling of shear modulus and spin-lattice relaxation time in $Ba(Fe,Co)_2As_2$

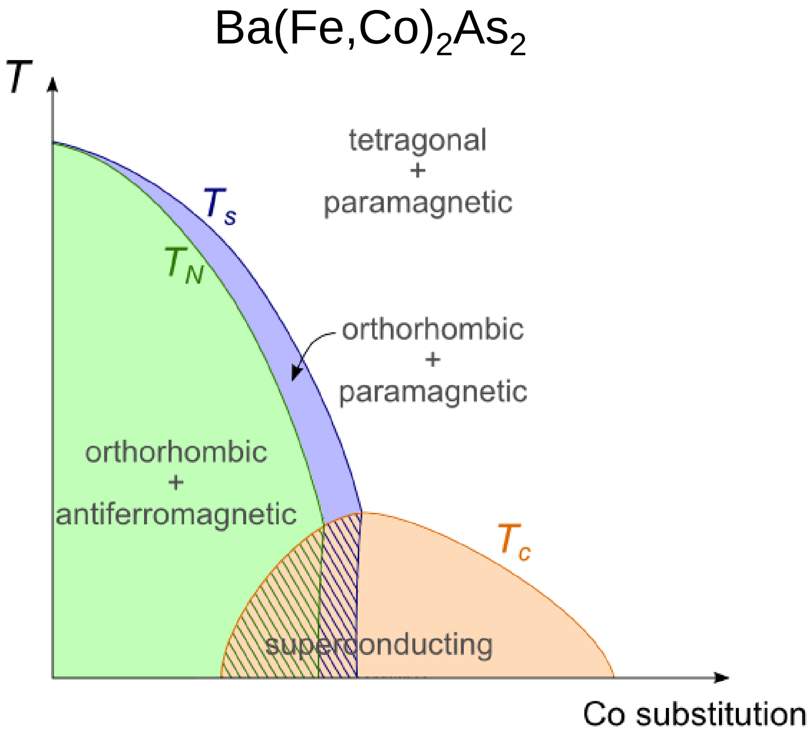
$$\frac{C_{66}}{C_{66,0}} = \frac{1}{1 + [a(T_1T) - b]^{-1}}$$

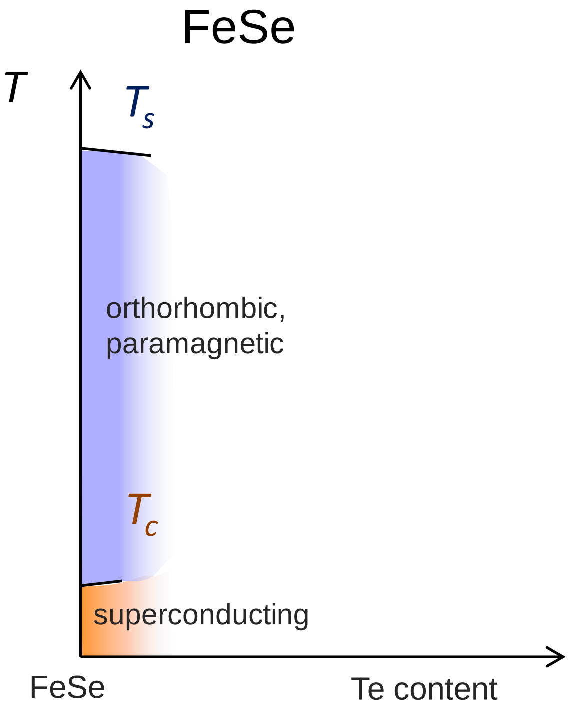


Evidence for magnetic origin of structural transition in $Ba(Fe,Co)_2As_2$

R. M. Fernandes et al., PRL 111, 137001 (2013)

The case of FeSe

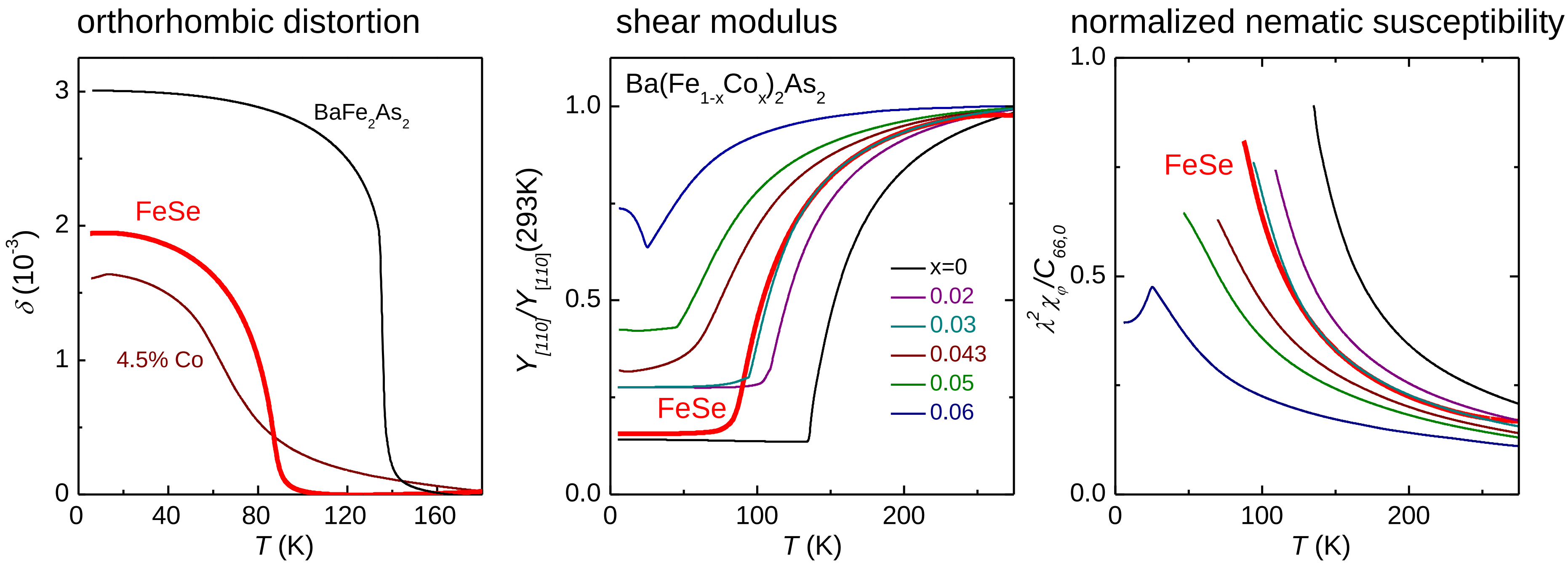




- Structural transition, analogous to $BaFe_2As_2$-systems, at ~90K
- No long range magnetic order at ambient pressure, emerges under pressure
- Superconducting below $T_c \sim 8\ \mathrm{K}$, huge increase of T_c under pressure

Is there a spin-nematic phase in FeSe?

The tetragonal-to-orthorhombic (nematic) transition: FeSe vs. $Ba(Fe,Co)_2As_2$



orthorhombic distortion

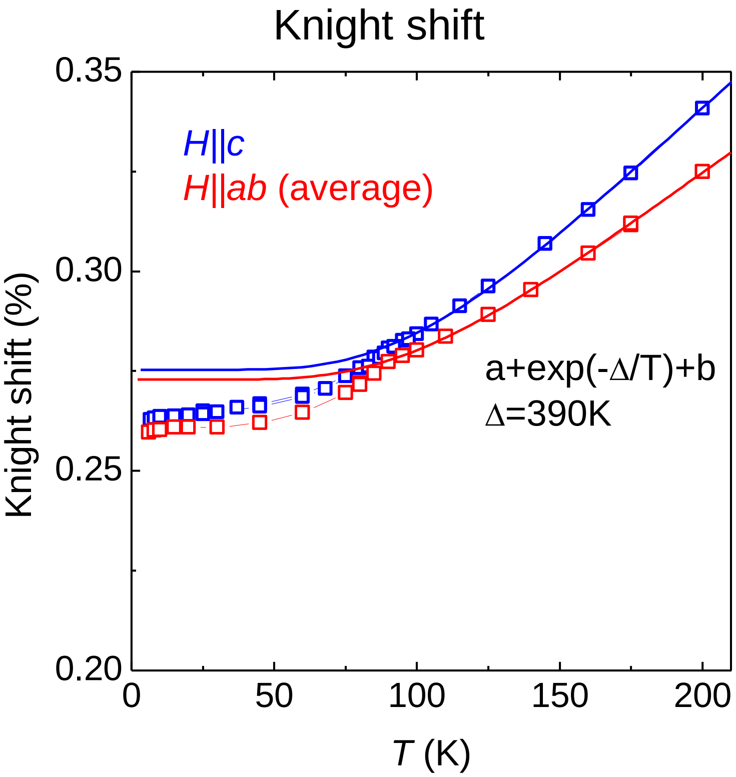
shear modulus

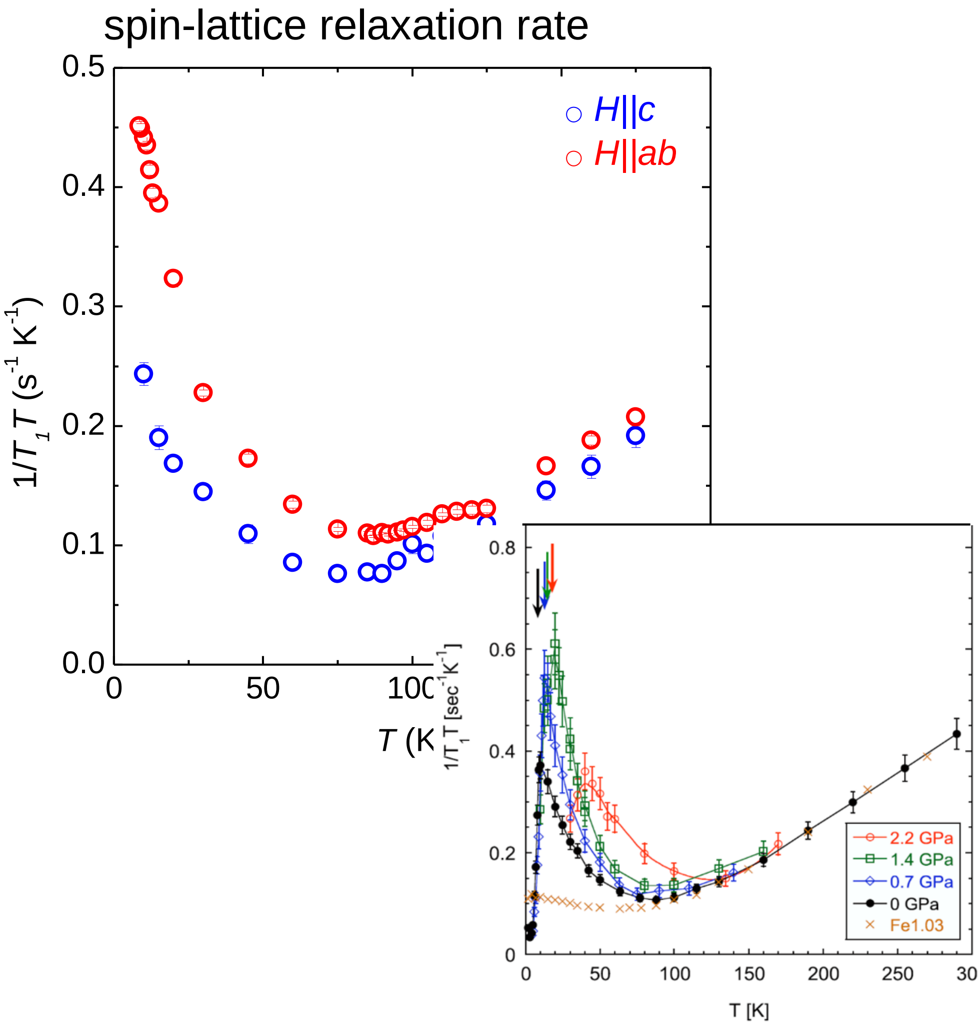
normalized nematic susceptibility

- Similar magnitude of orthorhombic distortion
- Nearly identical temperature dependence of the shear modulus:

  ⟹ same value of electron-lattice coupling?

NMR measurements on single-crystalline FeSe

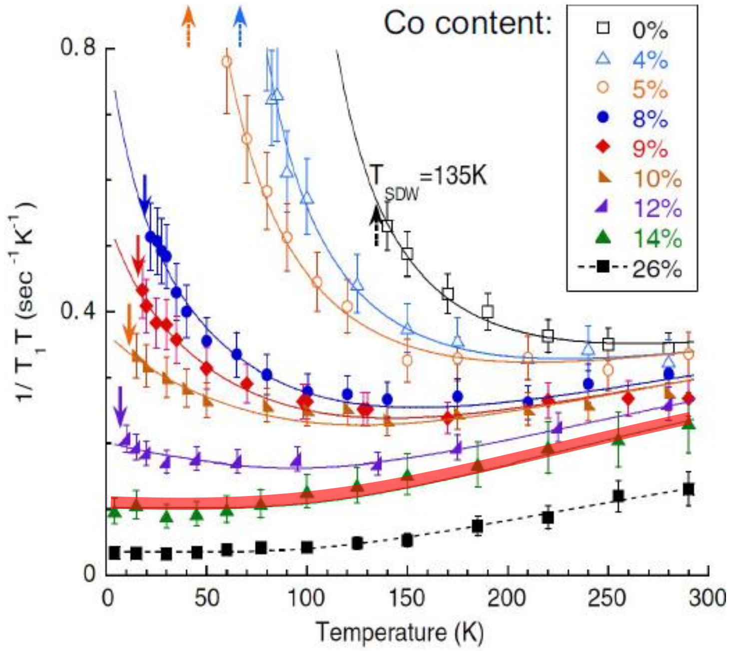




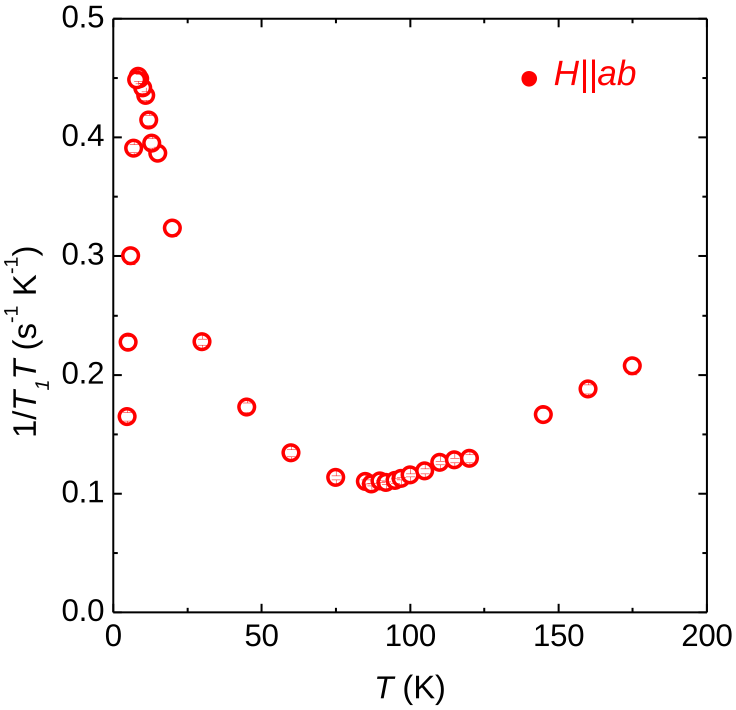
Imai et al., PRL 102, 177005 (2009)

Signature of spin fluctuations?

$Ba(Fe,Co)_2As_2$

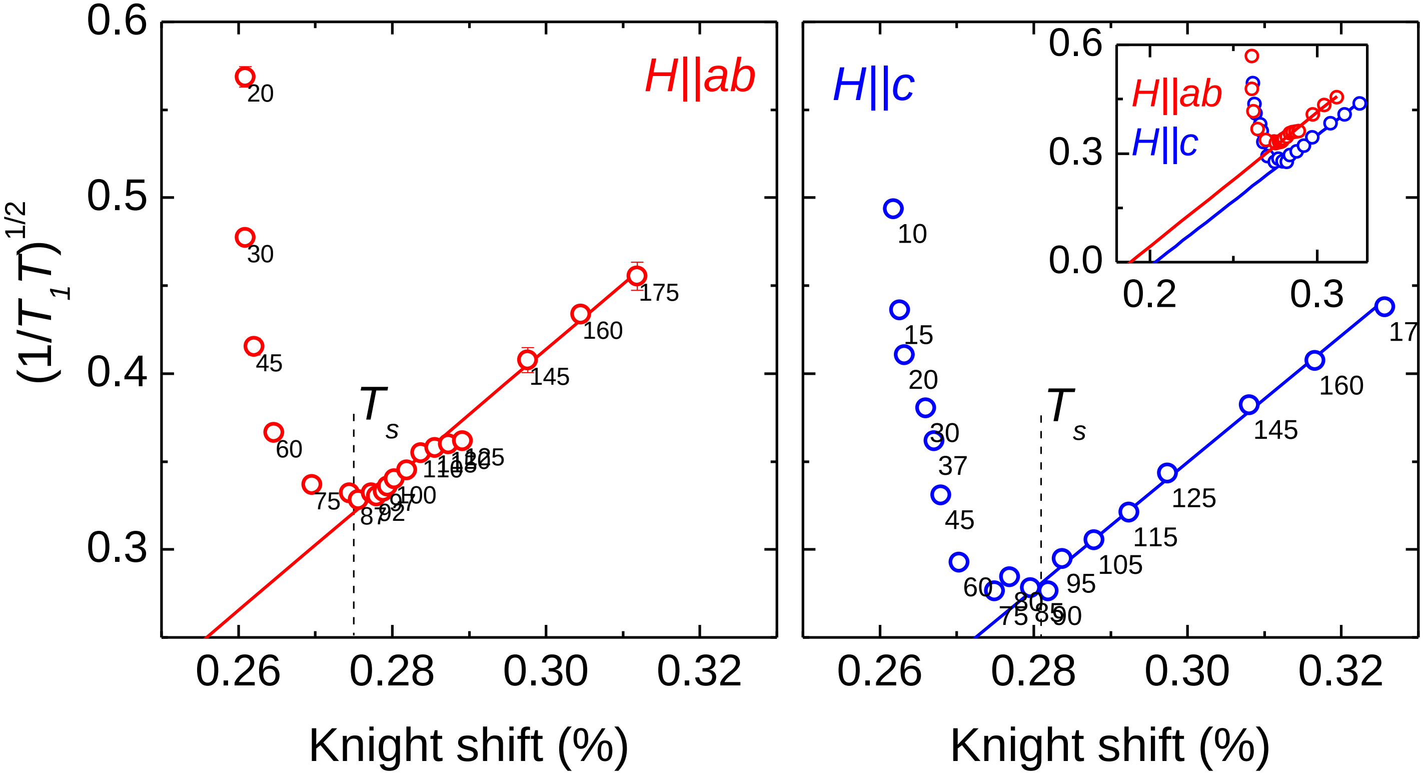


FeSe



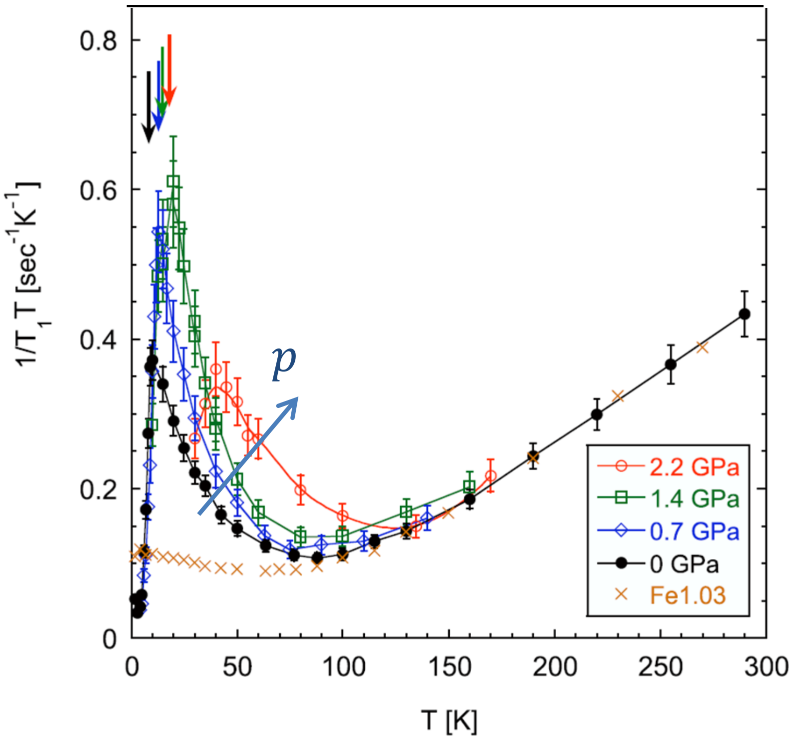
Analysis of the spin-lattice relaxation rate of FeSe

Korringa relation (Fermi liquid): $\left(\frac{1}{T_1 T}\right)^{1/2} \propto K + const.$

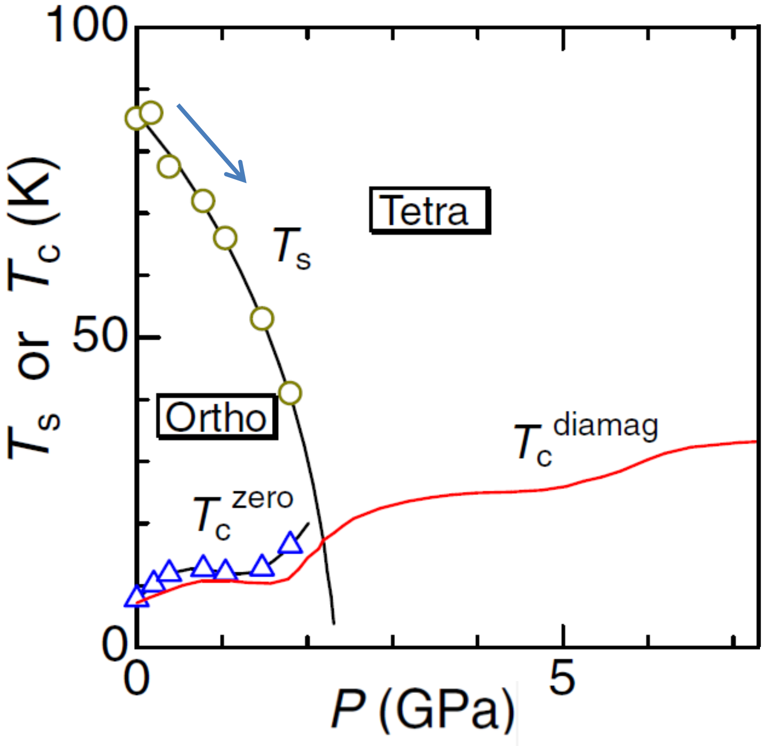


- Korringa relation is satisfied above T_s
- An additional contribution seems to emerge only below T_s

Does orbital order trigger magnetism in FeSe?



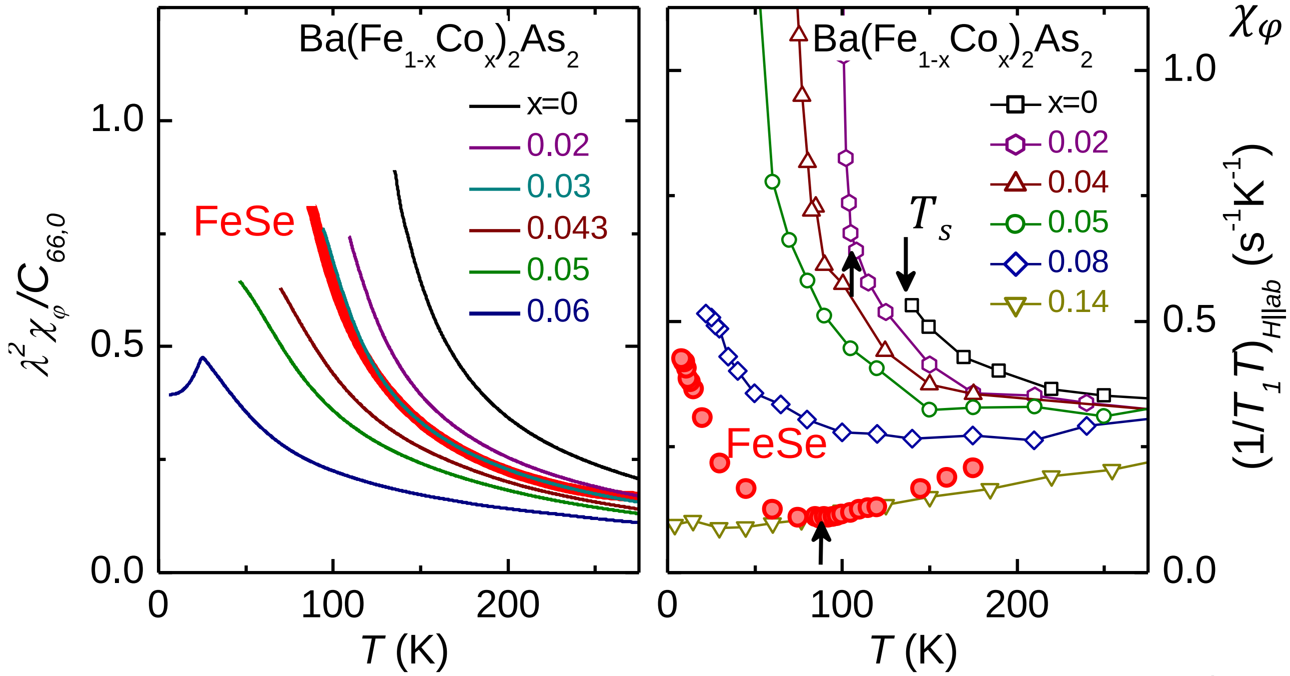
Imai et al., PRL 102, 177005 (2009)



Miyoshi et al., JPSJ 83, 013702 (2014)

- Pressure decreases T_s, but increases $1/T_1T$
- Magnetism and orthorhombic distortion appear to be independent in FeSe

Nematic susceptibility: FeSe vs. Ba(Fe,Co)$_2$As$_2$

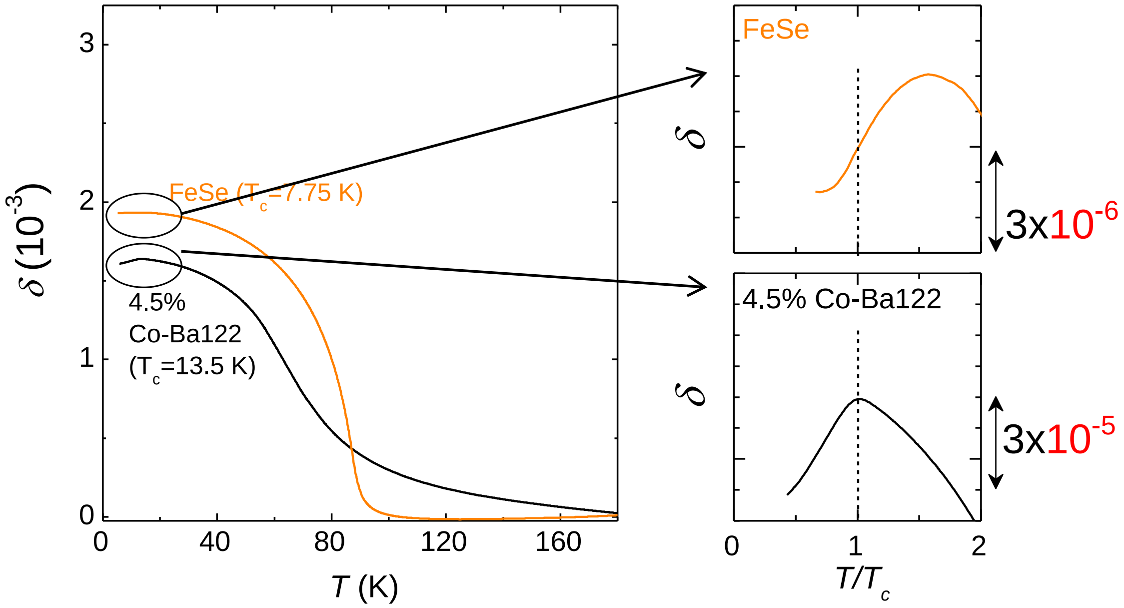


$$\chi_\varphi = \frac{\sum_q \chi^2(q)}{1 - g_0 \sum_q \chi^2(q)}$$

A. Böhmer, K. Ishida, C. Meingast et al., arxiv 1407.5497

- Same nematic susceptibility for FeSe and Ba(Fe,Co)$_2$As$_2$
- Magnetic fluctuations are only observed below T_s in NMR
- Magnetic fluctuations are an unlikely driving force for structural transition
- Is orbital ordering the origin for the structural transition in FeSe? (BaFe$_2$As$_2$?)

Lack of coupling between orthorhombic distortion and superconductivity in FeSe



A. Böhmer et al, PRB 87, 180505 (2013)

See e.g. Nandi et al. PRL 2010

- No reduction of orthorhombic distortion below T_c
- $\Rightarrow dT_c/dp_a = dT_c/dp_b$

Conclusions

- The nematic susceptibility can be extracted from shear-modulus measurements
- Quantum-critical-like behavior in $Ba(Fe,Co)_2As_2$, but a first-order transition between different ground states in $(Ba,K)Fe_2As_2$
- Magnetic fluctuations can explain the structural transition in $Ba(Fe,Co)_2As_2$, but not in FeSe

Magnetism without distortion
and
distortion without magnetism:

Relationship between nematicity and magnetism in Fe-based superconductors remains open …
?