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2 - 13 August 2010

What we have Learned from Ba(Fe1-xTMx)2As2 studies: Empirical rules to inform theory

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What we have learned from $Ba(Fe_{1-x}TM_x)_2As_2$ studies: empirical rules to inform theory

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August 2010

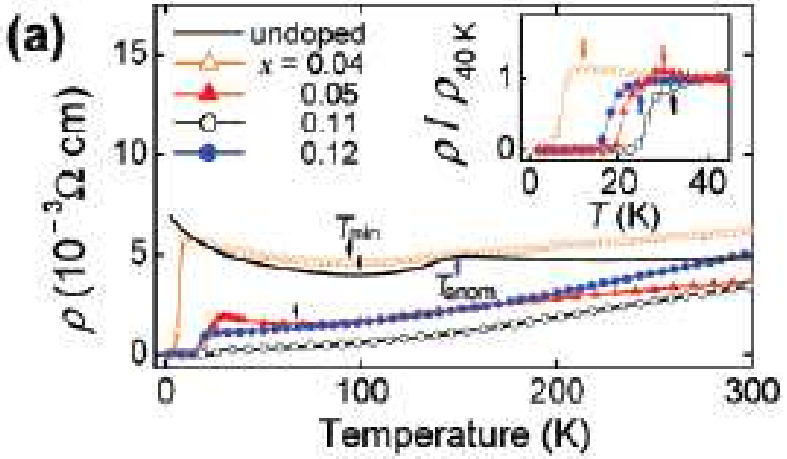
Trieste, Italy

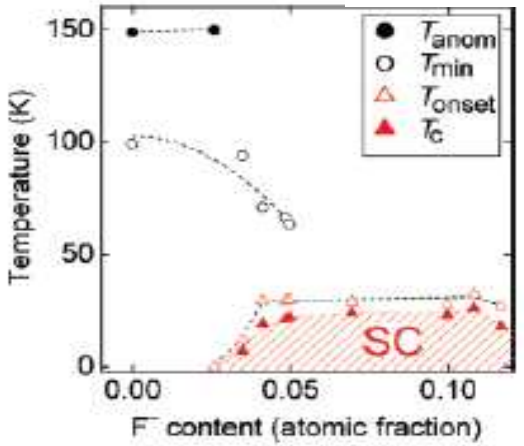
Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

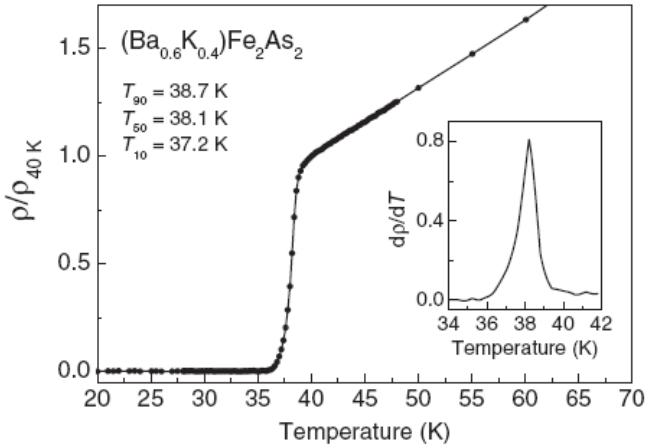




Superconductivity at 38 K in the Iron Arsenide $(Ba_{1-x}K_x)Fe_2As_2$

(Received 29 May 2008; published 5 September 2008)

Marianne Rotter, Marcus Tegel, and Dirk Johrendt*



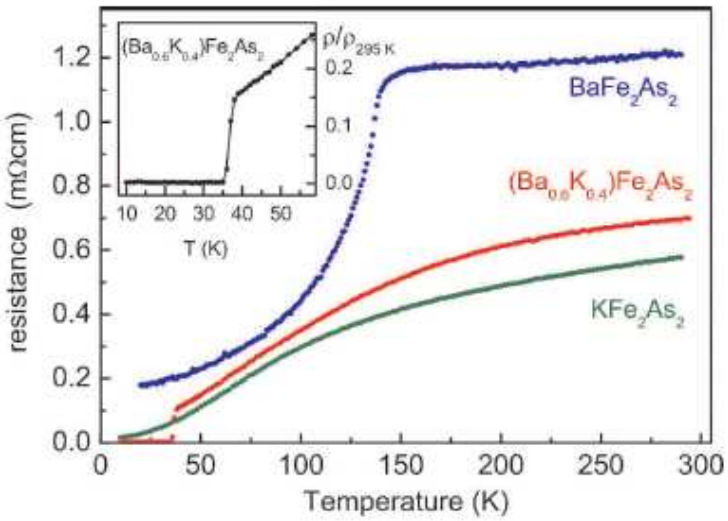


FIG. 4. Resistivity transition of $(Ba_{0.6}K_{0.4})Fe_2As_2$.

Co-doping can be used to stabilize T_c!!

PHYSICAL REVIEW B 78, 104505 (2008)

Superconductivity in $LaFe_{1-x}Co_xAsO$

(Received 6 July 2008; revised manuscript received 4 August 2008; published 10 September 2008)

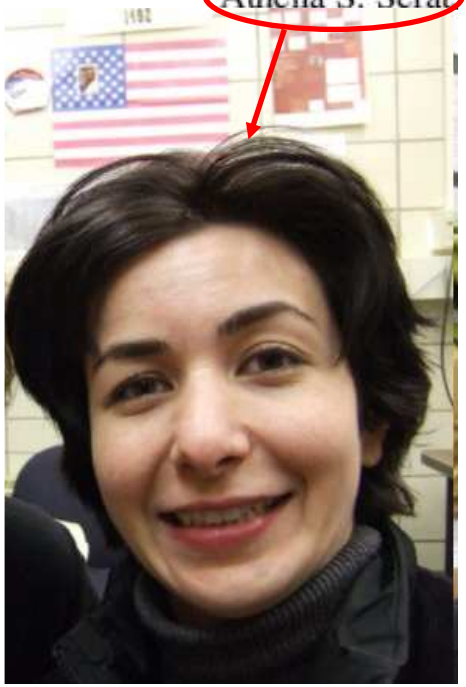
Athena S. Sefat,[1] Ashfia Huq,[2] Michael A. McGuire,[1] Rongying Jin,[1] Brian C. Sales,[1] David Mandrus,[1] Lachlan M. D. Cranswick,[3] Peter W. Stephens,[4] and Kevin H. Stone[4]

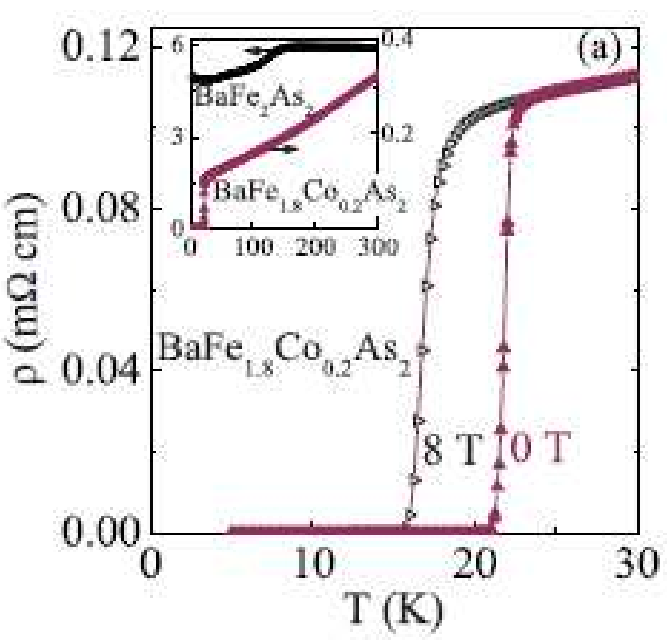
PRL 101, 117004 (2008) PHYSICAL REVIEW LETTERS week ending 12 SEPTEMBER 2008

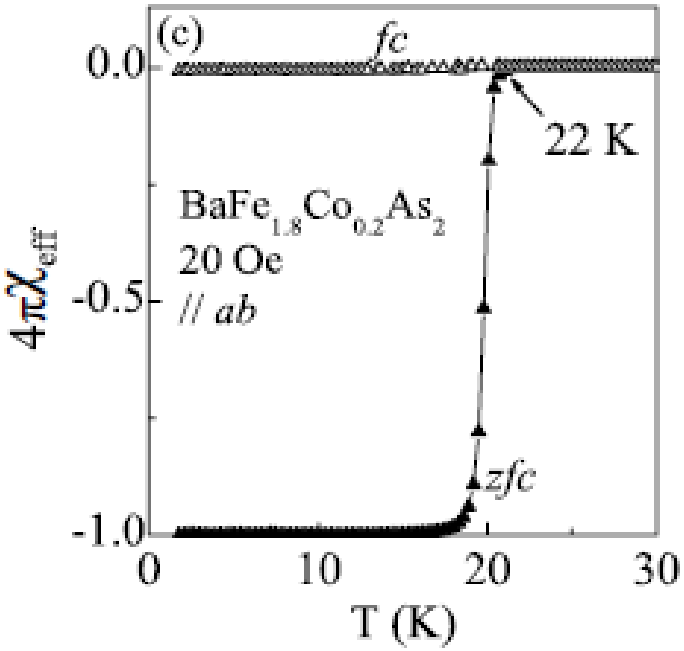
Superconductivity at 22 K in Co-Doped $BaFe_2As_2$ Crystals

Athena S. Sefat, Rongying Jin, Michael A. McGuire, Brian C. Sales, David J. Singh, and David Mandrus

(Received 25 July 2008; published 11 September 2008)







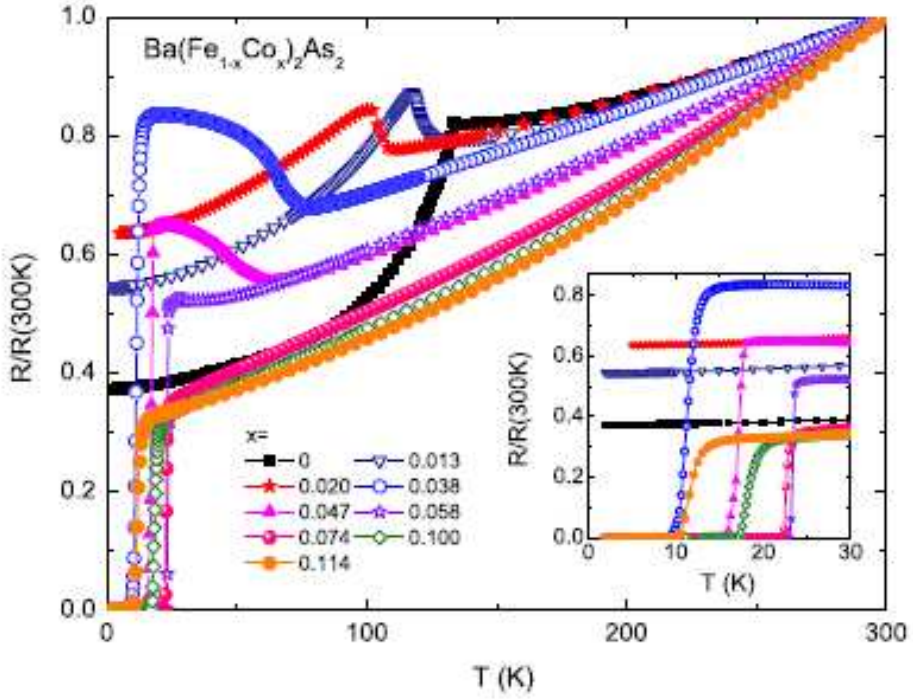
Doping of $BaFe_2As_2$ (or $SrFe_2As_2$) on the Fe site with transition metals (TM) is important for two basically different reasons: (i) very different from CuO-based superconductors, (ii) offered easier and more homogeneous doping than K- or other alkali-doping.

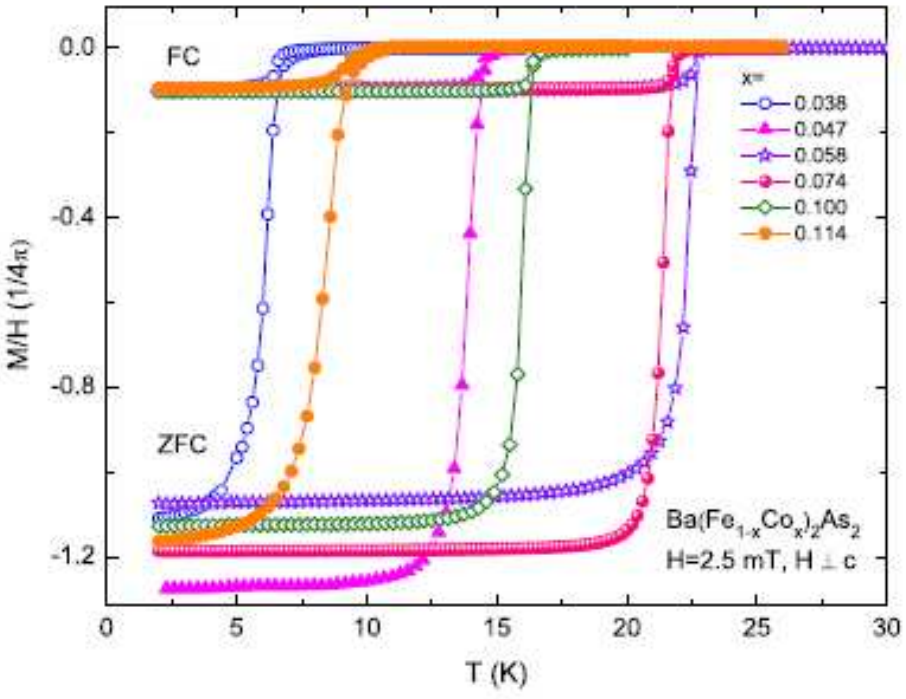
PHYSICAL REVIEW B 78, 214515 (2008)

Effects of Co substitution on thermodynamic and transport properties and anisotropic H_{c2} in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals

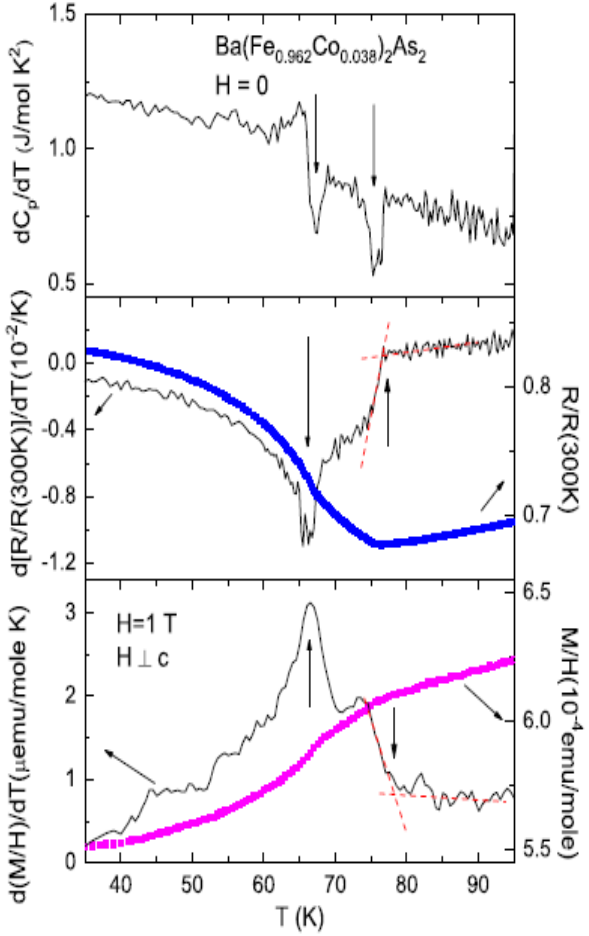
N. Ni,[1] M. E. Tillman,[1] J.-Q. Yan,[1] A. Kracher,[1] S. T. Hannahs,[2] S. L. Bud'ko,[1] and P. C. Canfield[1]

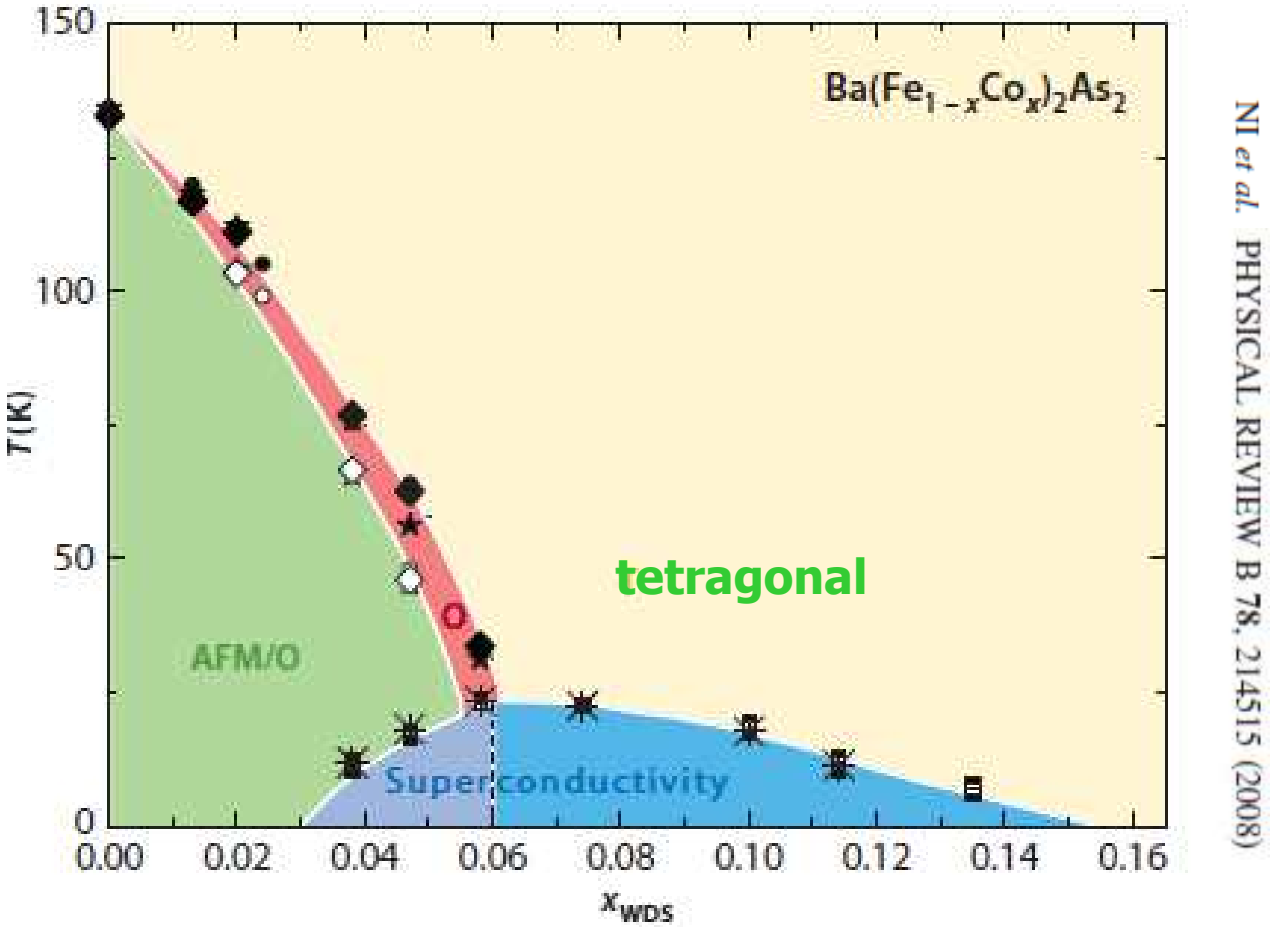
(Received 11 November 2008; published 29 December 2008)





Using thermodynamic and transport data we could assemble a T-x phase diagram that clearly showed (i) superconducting dome existing in both ortho/AF and tetragonal phases and (ii) a splitting (or broadening) of the x = 0 simultaneous orthorhombic and antiferromagnetic phase transition.





NI *et al.* PHYSICAL REVIEW B 78, 214515 (2008)

Oh no, I hear one of our organizers chiding me

"Wait, my dear fellow, you are not adequately abiding by our traditions of pedagogy and stately discussion…."

Also remember to pack a towel

10-15 mins pedagogical intro

In my research group we try to think, make, measure, think

Each of these steps has its own subtleties and difficulties

Make:

How are samples made and what quality assurance is needed / done?

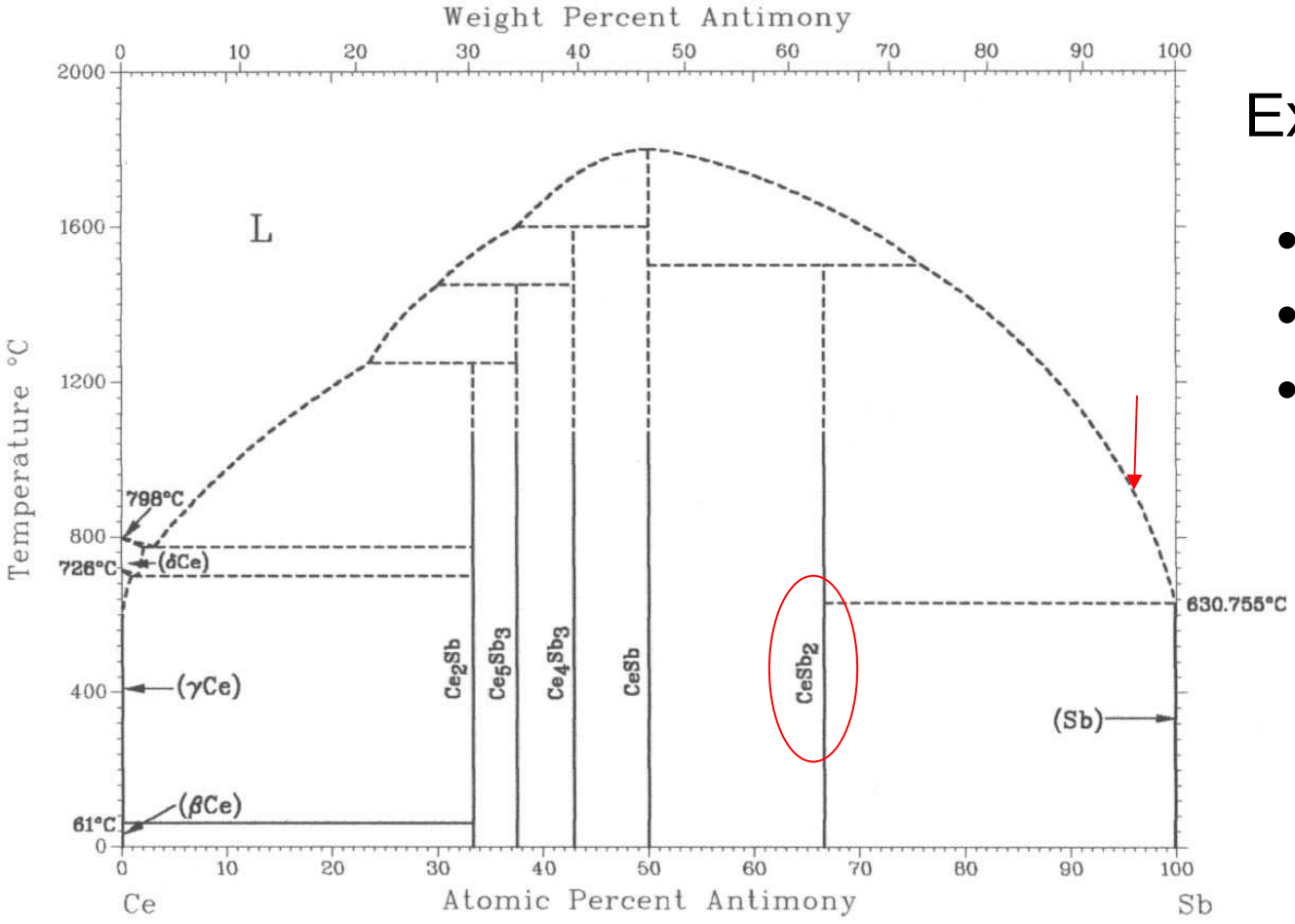
Measure:

How are phase diagrams such as these assembled and what assumptions / sins are committed in their formation?

Thinking we will discuss later….

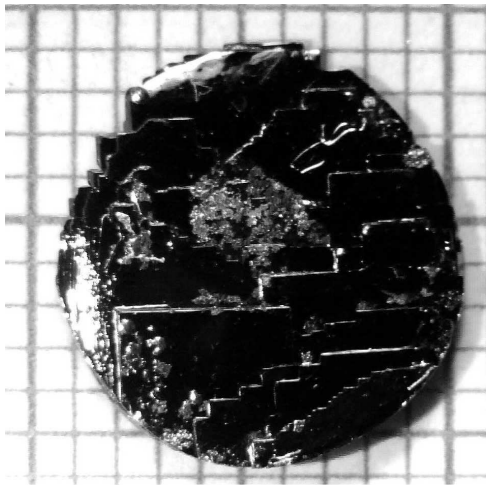
The single crystalline samples were grown out of a flux (slow cooling of a melt)

Basic idea: slow cool into 2-phase region



Example: $CeSb_2$ / Sb

- self flux
- $Ce_{0.05}Sb_{0.95}$
- 1190 ℃ → 700 ℃

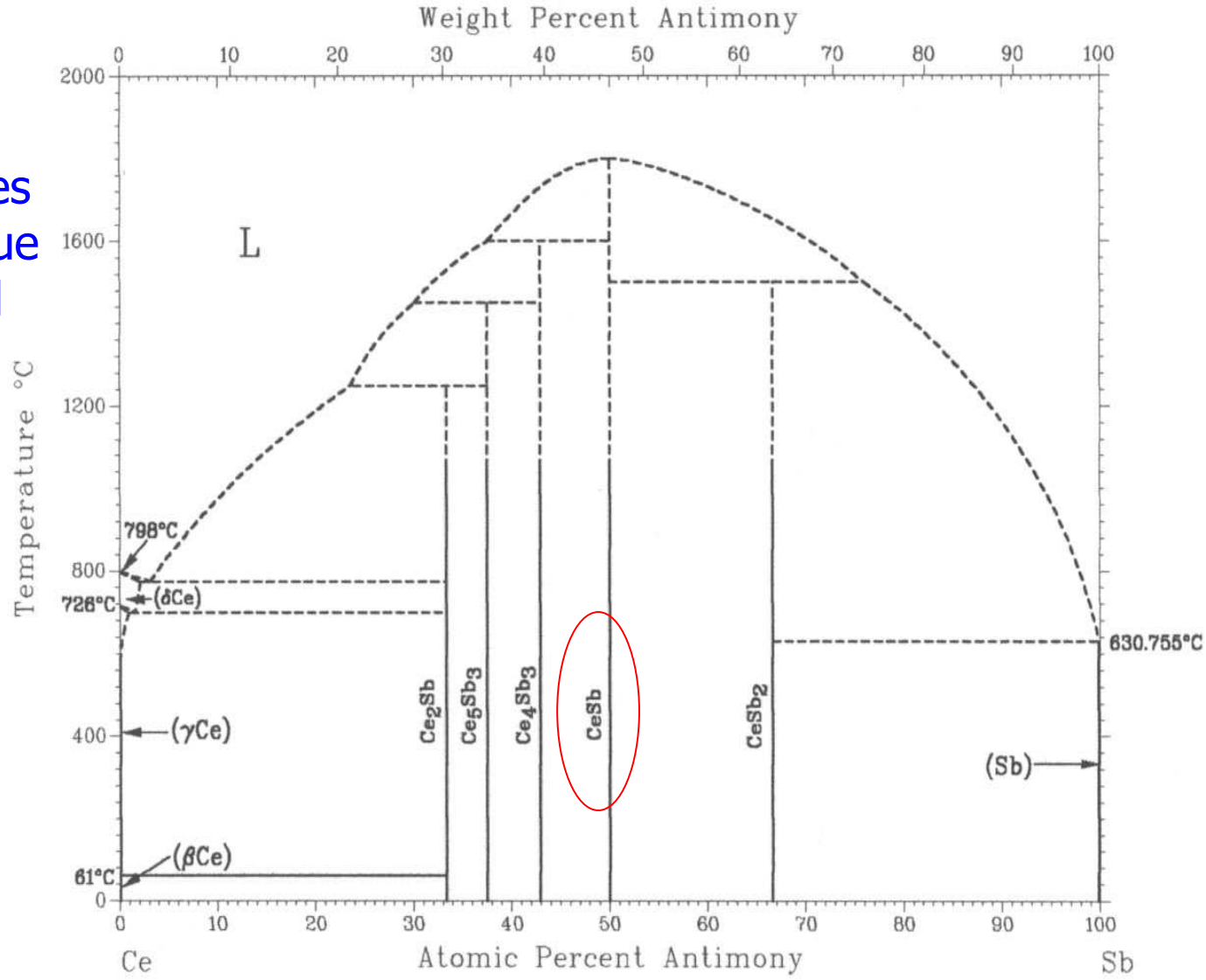


What about more difficult growths, such as CeSb?

This is tricky if done just out of the binary: very high temperatures and lots of defects (due to vapor pressure and entropy).

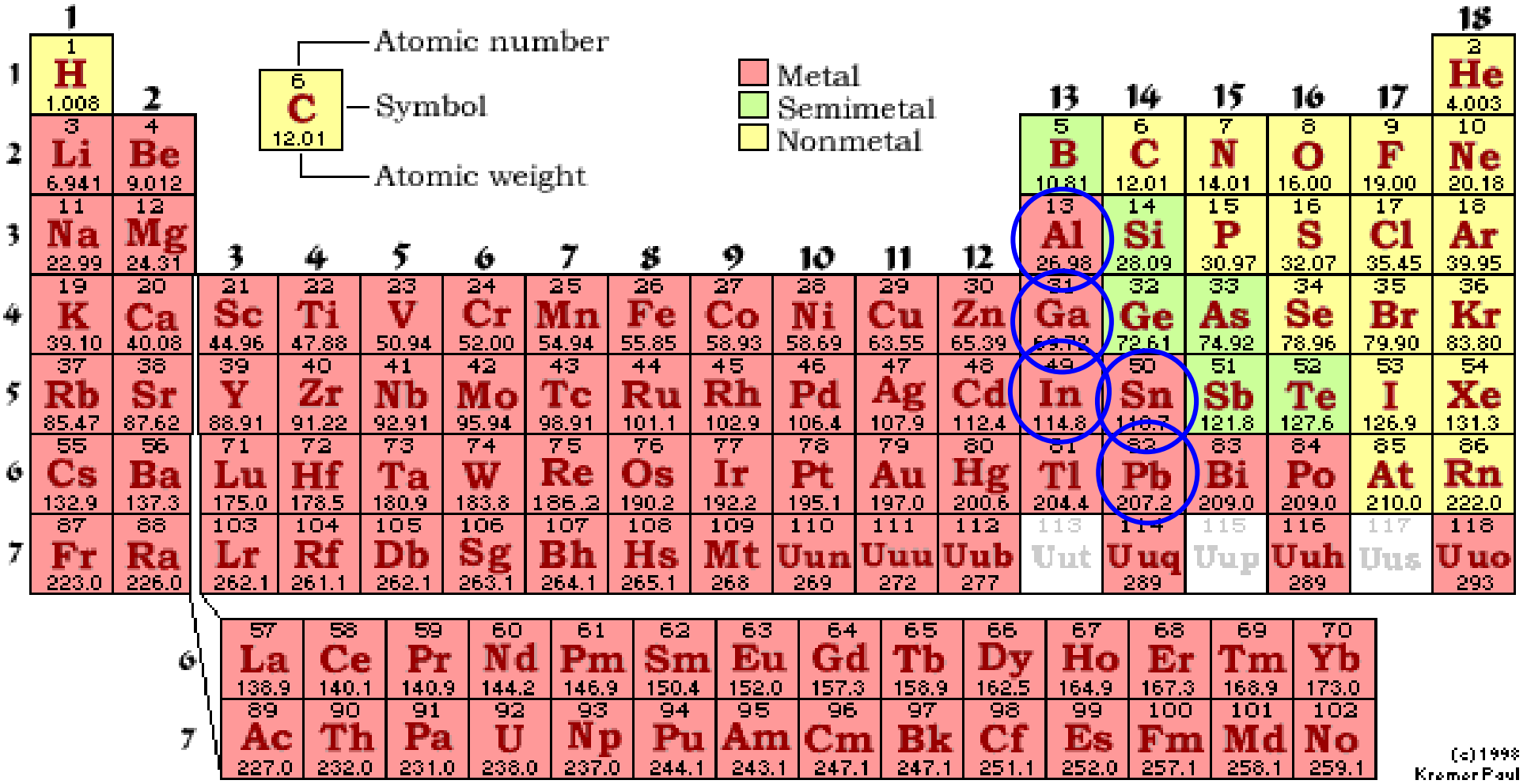
Can this be grown out of extra elements in manner similar to growing a salt out of water?

This question is the essence of flux growth.

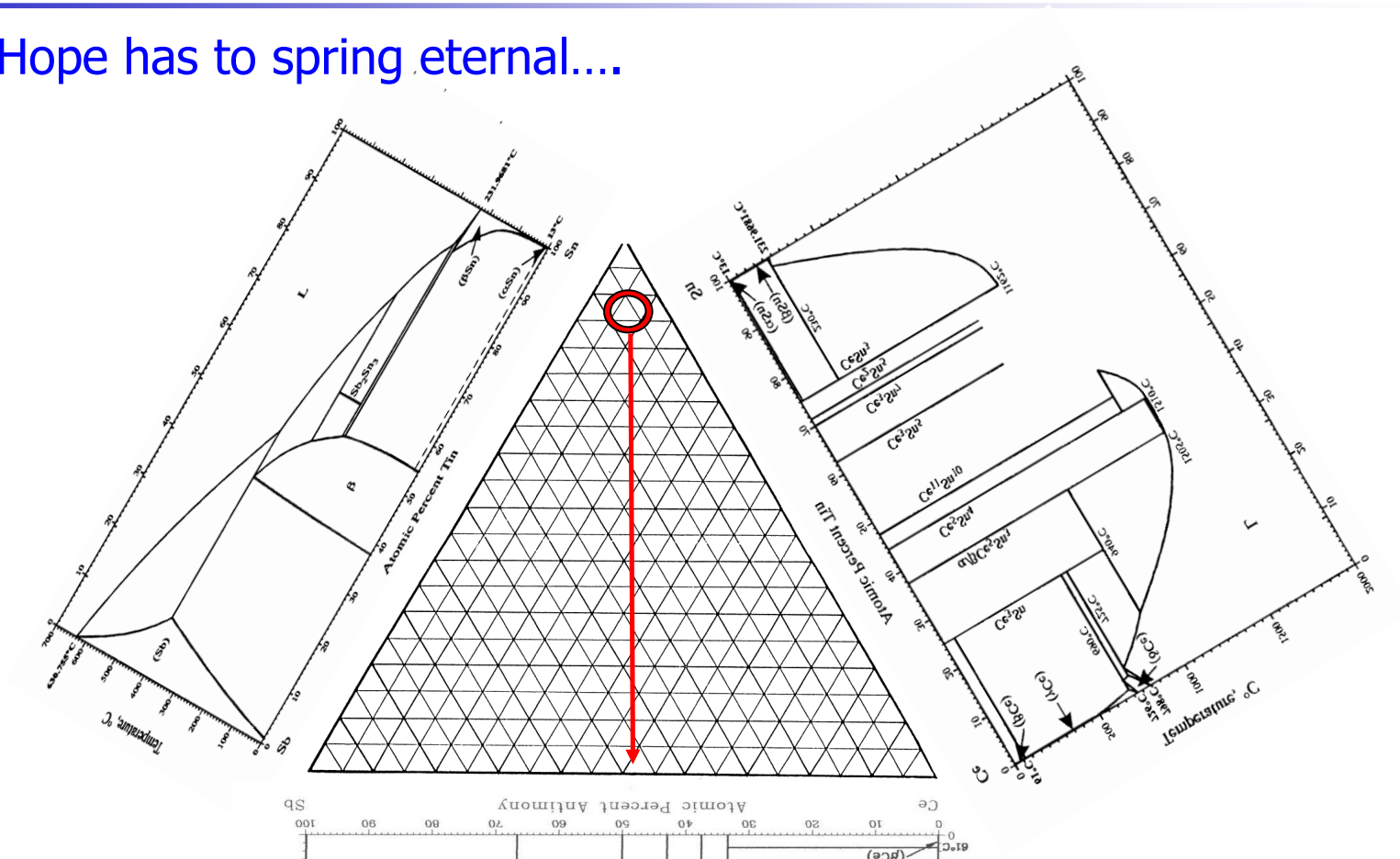


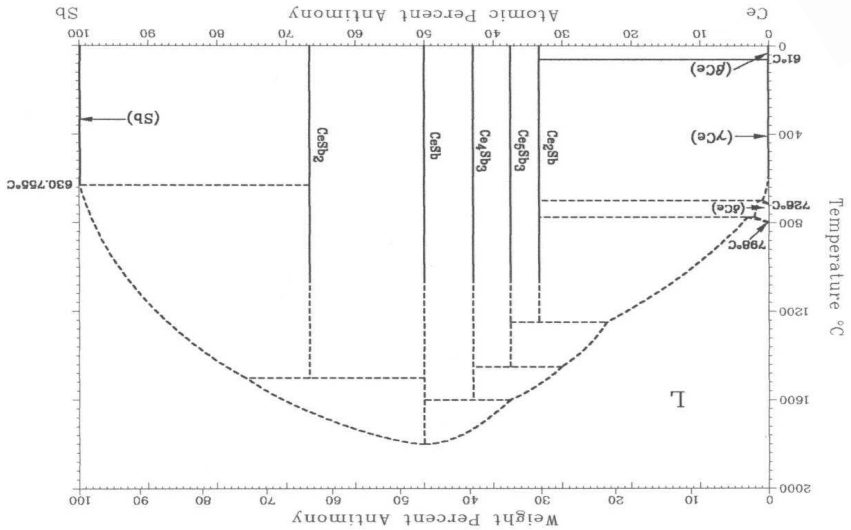
When I was first faced with this goal I simply tried several of the "usual suspects", i.e. low melting elements that offered good solubility for both Ce and Sb.

Sn worked best



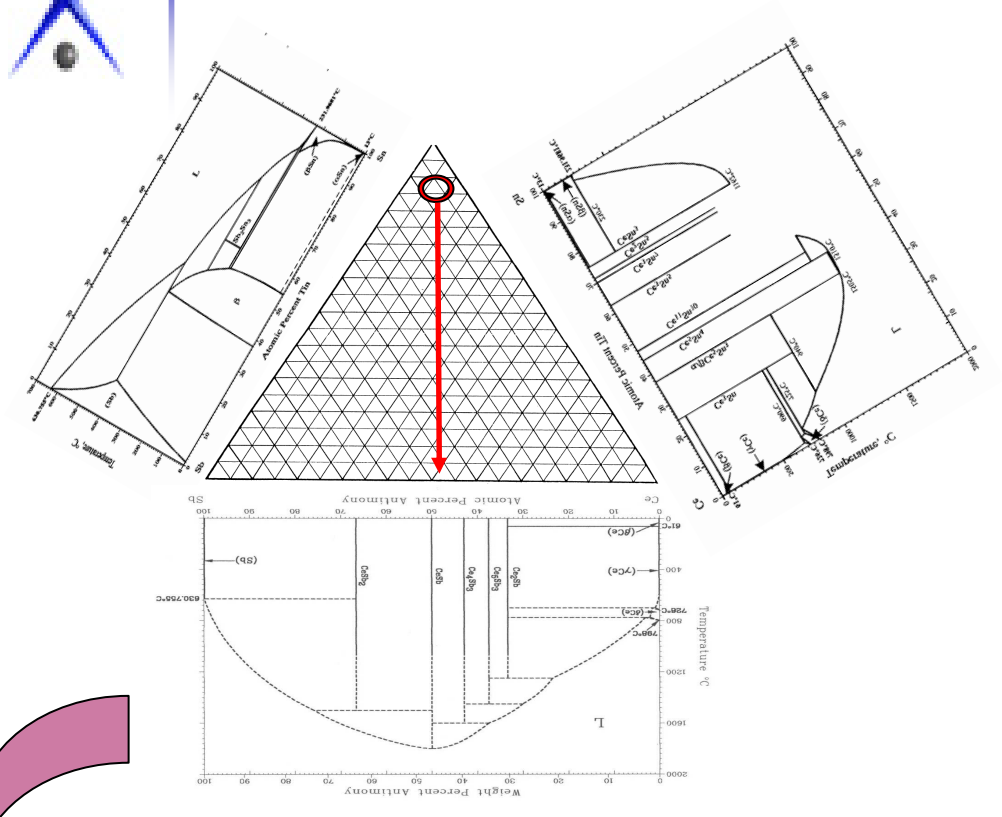
Hope has to spring eternal….





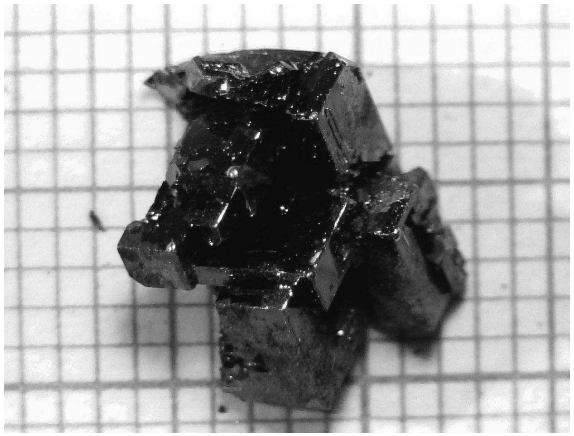
The hope is that CeSb can be grown out of a vast excess of Sn

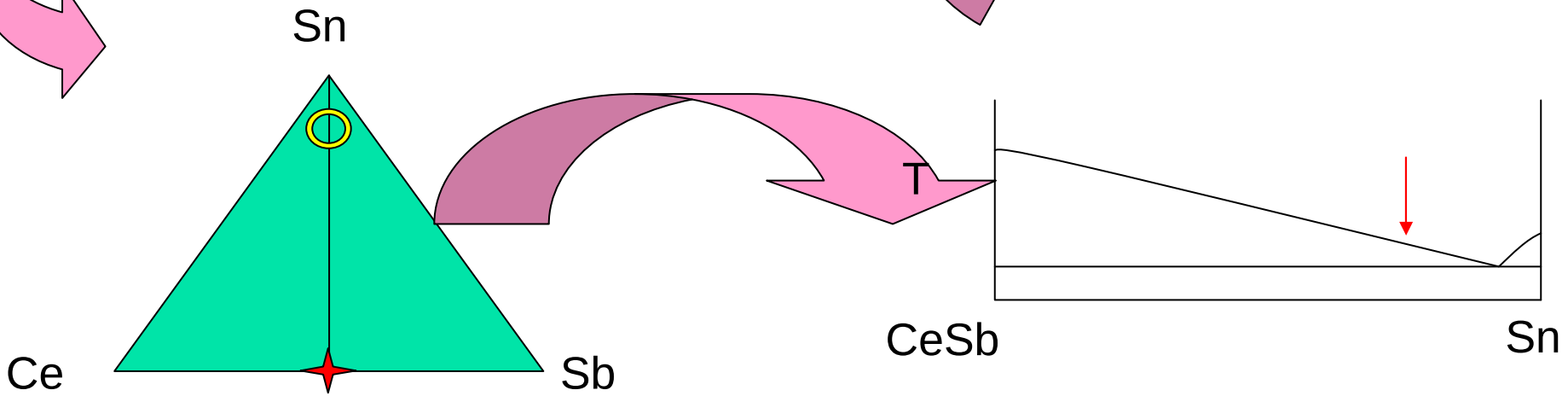
This is the same hope that allows you to grow single crystals of various salts and sugars out of water.



$(CeSb)_{0.05}Sn_{0.95}$

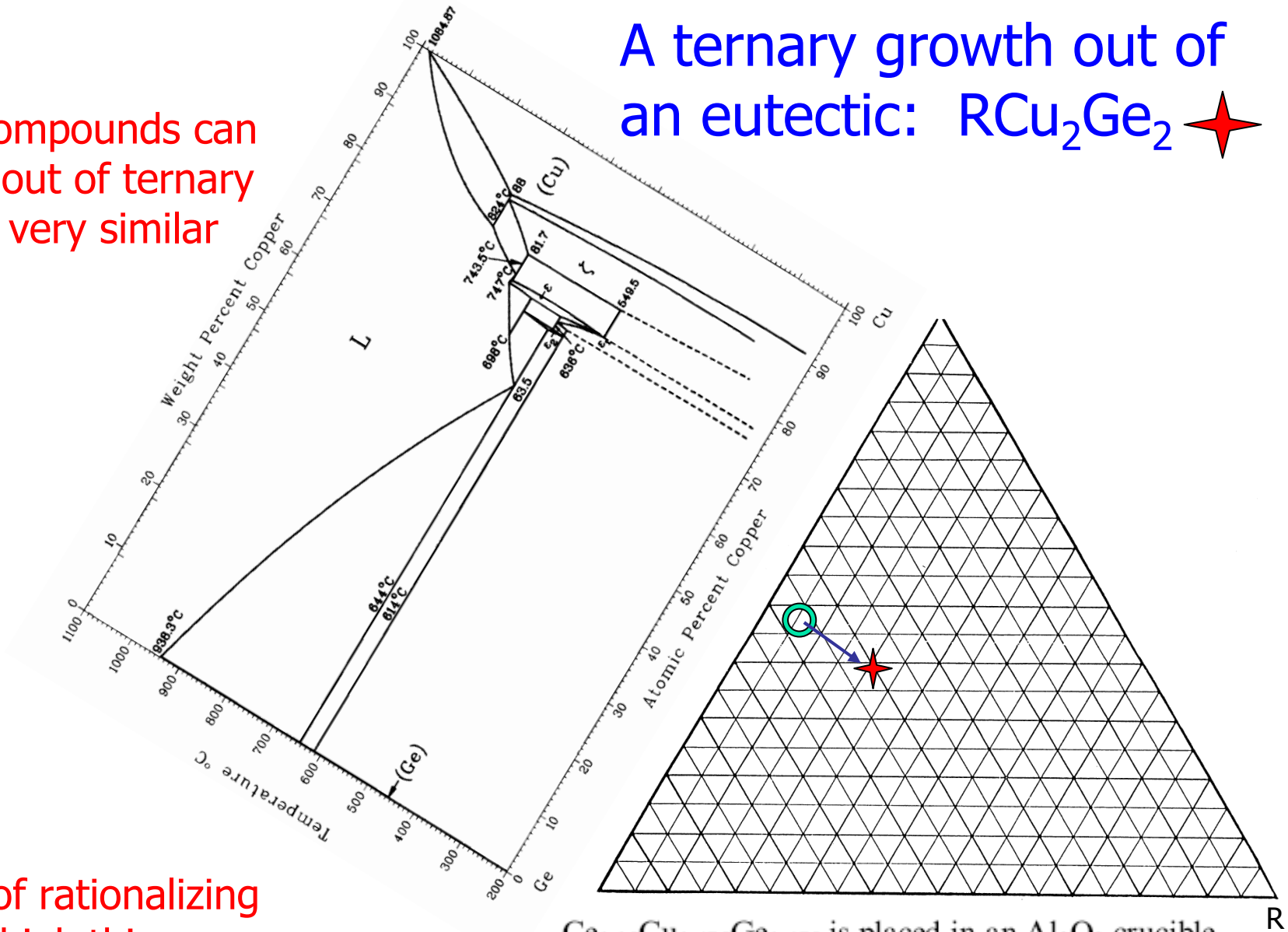
1100 ℃ → 800 ℃





A ternary growth out of an eutectic: RCu_2Ge_2

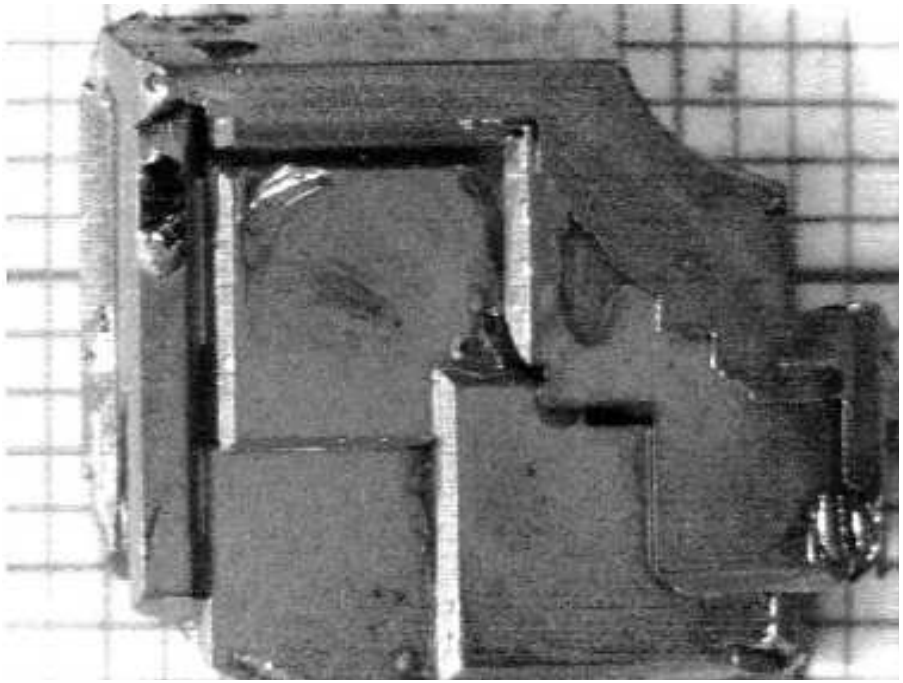
Ternary compounds can be grown out of ternary melts in a very similar manner.



One way of rationalizing this is to think this as "perturbation" of the binary

$Ce_{0.05}Cu_{0.475}Ge_{0.475}$ is placed in an Al_2O_3 crucible, sealed in a quartz ampule and heated to 1190°C. The ampule is cooled to 825°C over 200 h and then the excess liquid is decanted. The resulting crystal

$CeCu_2Ge_2$ (m = 2 g)



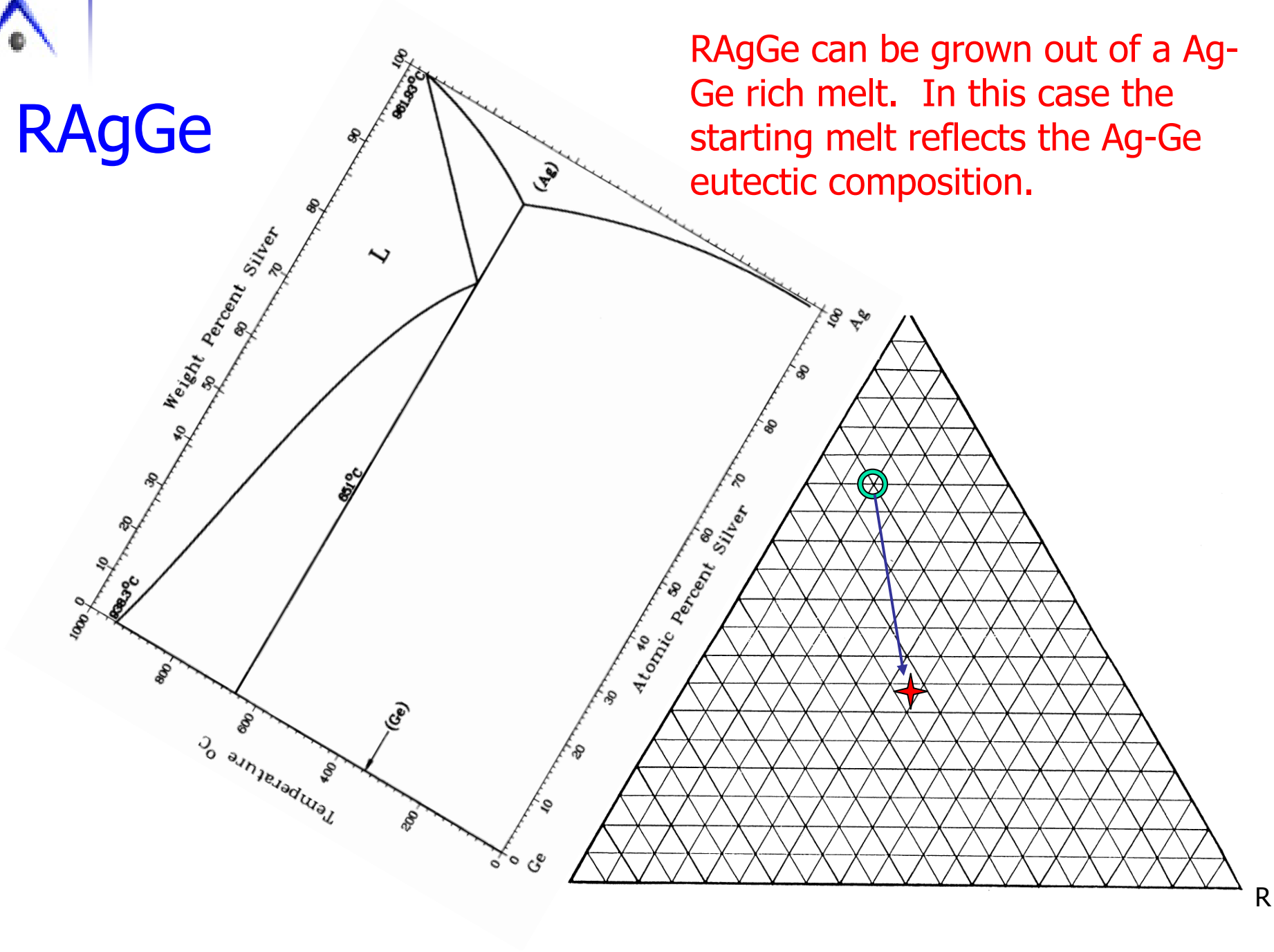
Grown in a 5 ml Al_2O_3 crucible, sealed in silica

200 hours

1190 C → 825 C

RAgGe

RAgGe can be grown out of a Ag-Ge rich melt. In this case the starting melt reflects the Ag-Ge eutectic composition.

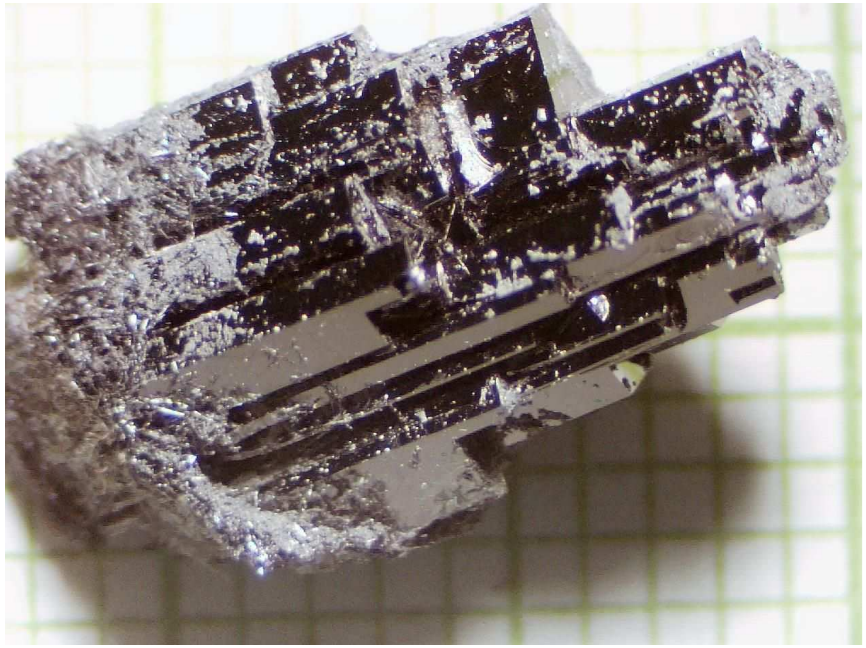


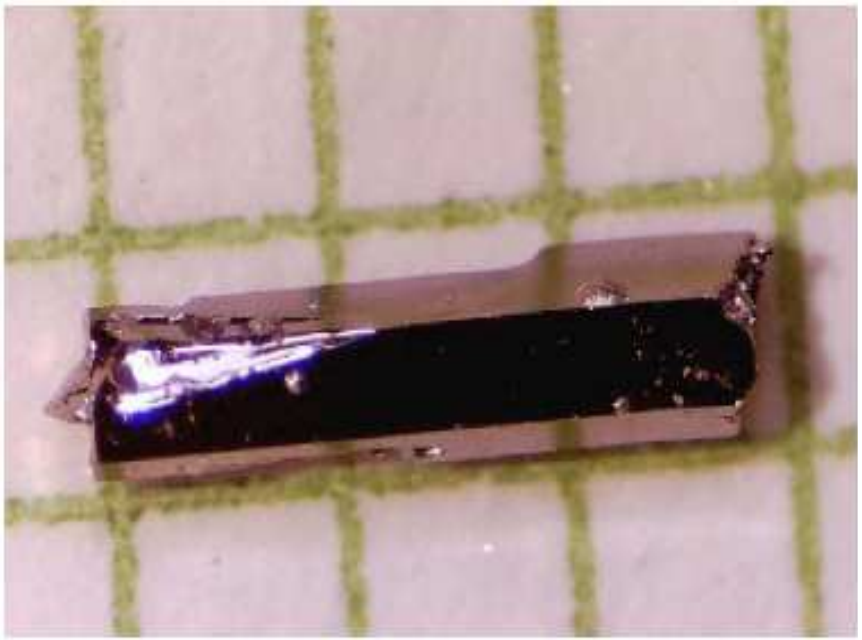
R

Melt stoichiometry: $Yb_{10}Ag_{68}Ge_{22}$

1100 C $\xrightarrow{100\ hr}$ 850 C

Crystals of RAgGe have allowed for the study of anisotropic metamagnetism as well as the discovery of new quantum critical properties in YbAgGe.

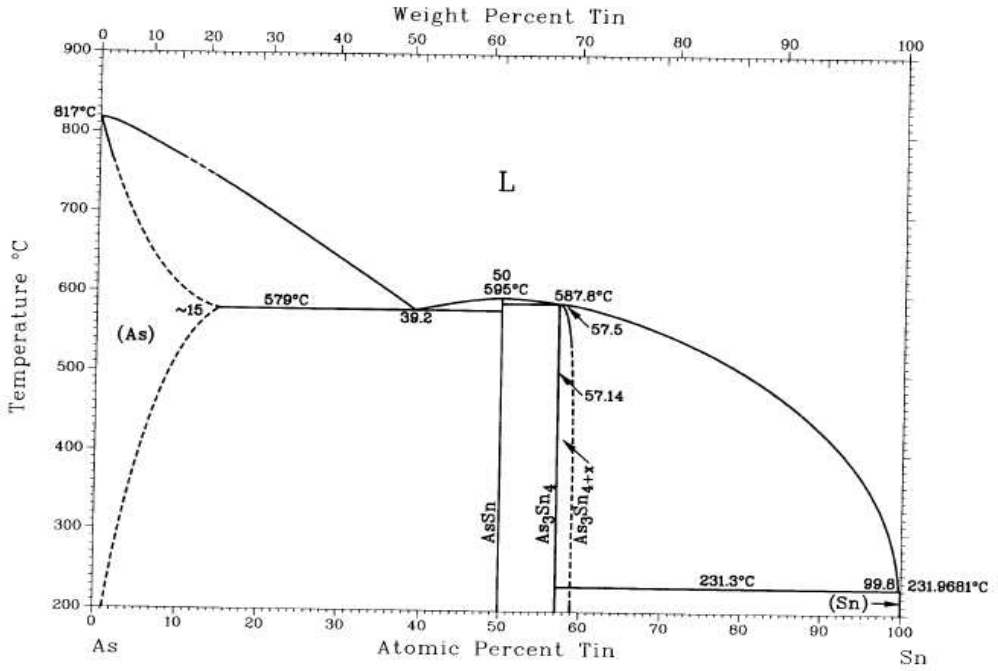




Similar growth techniques have been applied to the AFe_2As_2 (A = Ba, Sr, Ca) families of compounds.

Over the decades we have used Sn as very powerful flux for the growth of many intermetallic compounds: RSb, various $R(TM)_2Ge_2$ and $R(TM)_2Si_2$ compounds, $Yb_{14}MnSb_{11}$ and other compounds. *Within 14 hours of hearing about superconductivity in K-doped $BaFe_2As_2$ we had grown the first single crystals out of a Sn-rich quaternary melt.*

Sn has the distinct advantage of allowing the use of As more safely given that in a Sn solution the vapor pressure is held down.



With Sn growth we opened the AFe_2As_2 compound up for study. The samples are well formed, but a bit small.

PHYSICAL REVIEW B 78, 014507 (2008)

Anisotropic thermodynamic and transport properties of single-crystalline $Ba_{1-x}K_xFe_2As_2$ ($x=0$ and 0.45)

N. Ni,[1,2] S. L. Bud'ko,[1,2] A. Kreyssig,[1,2] S. Nandi,[1,2] G. E. Rustan,[1,2] A. I. Goldman,[1,2] S. Gupta,[1,3] J. D. Corbett,[1,3] A. Kracher,[1] and P. C. Canfield[1,2]

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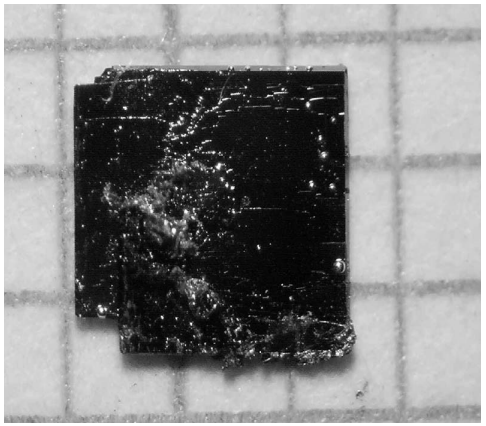

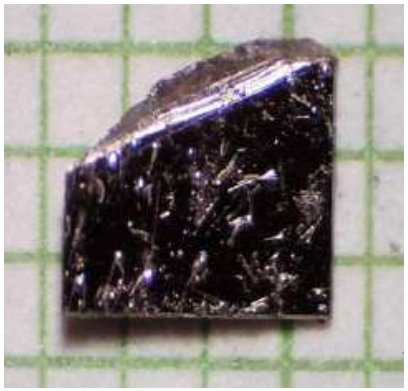

PHYSICAL REVIEW B 78, 024516 (2008)

Structural transition and anisotropic properties of single-crystalline $SrFe_2As_2$

J.-Q. Yan,[1] A. Kreyssig,[1,2] S. Nandi,[1,2] N. Ni,[1,2] S. L. Bud'ko,[1,2] A. Kracher,[1] R. J. McQueeney,[1,2] R. W. McCallum,[1,3] T. A. Lograsso,[1] A. I. Goldman,[1,2] and P. C. Canfield[1,2]

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PHYSICAL REVIEW B 78, 014523 (2008)

First-order structural phase transition in $CaFe_2As_2$

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Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

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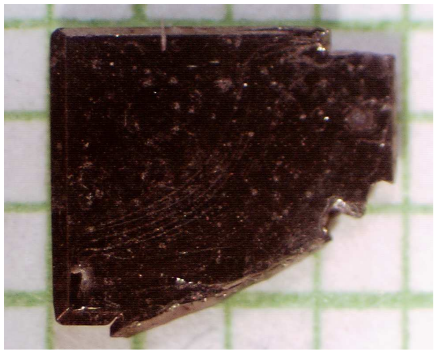


Substitution can never be taken for granted. What you put in is not necessarily what comes out.

The substitution of K for Ba or Sr in the AFe_2As_2 materials is difficult, due to a combination of vapor pressure and reactivity, and can lead to compositional inhomogeneities. This is a problem for crystal grown from Sn as well as those grown from FeAs.

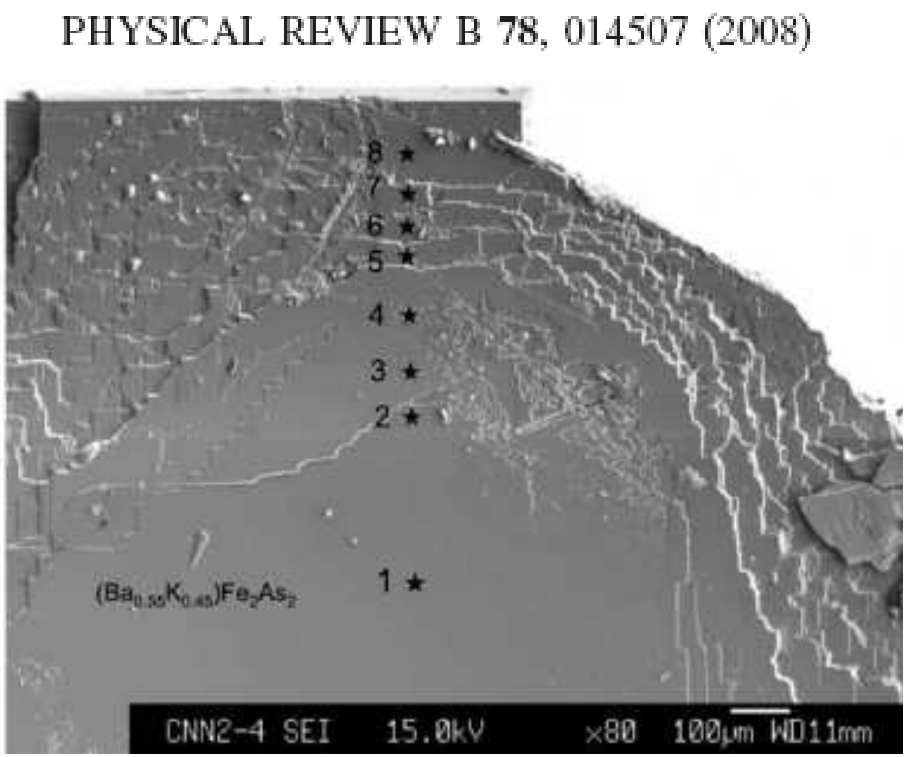


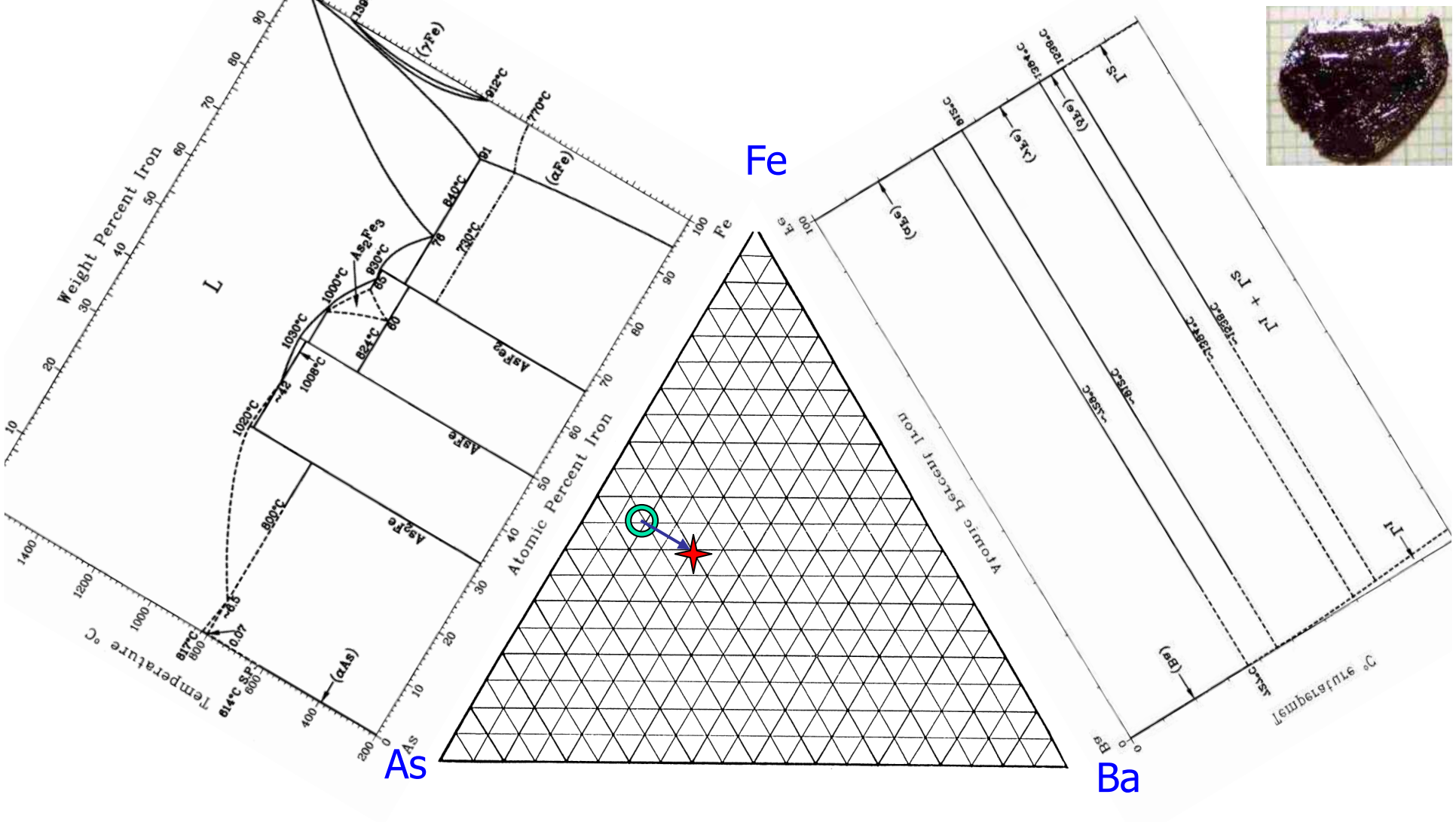
TABLE I. WDS elemental analysis (in atomic %) for $Ba_{0.55}K_{0.45}Fe_2As_2$ single crystal shown in Fig. 2.

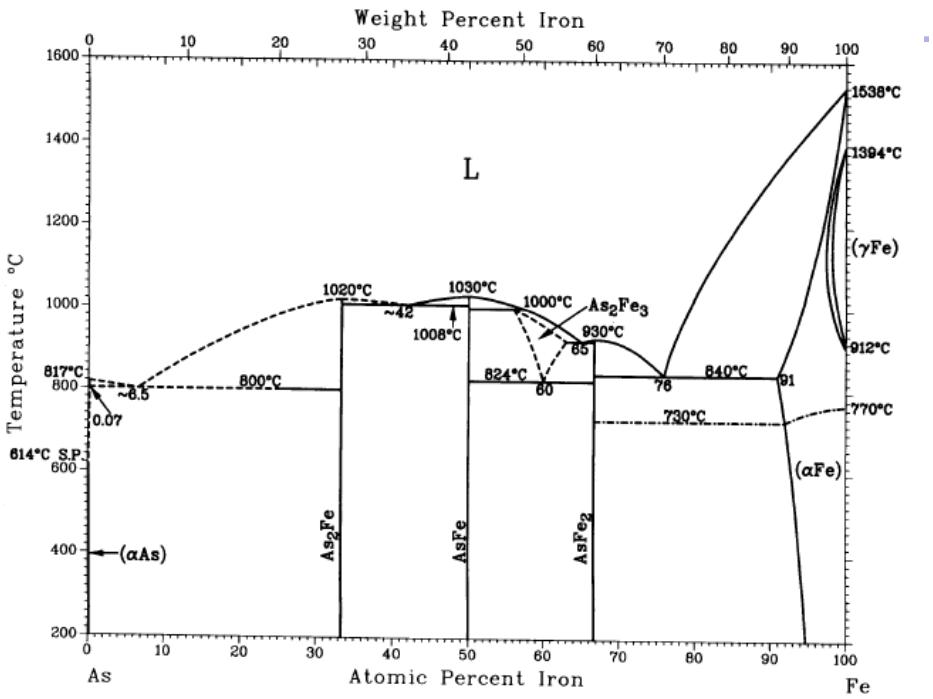
Point	As	Sn	K	Fe	Ba	K/(K+Ba)
1	37.6	0.53	10.2	41.7	9.9	0.51
2	38.5	0.74	8.1	40.3	12.3	0.40
3	38.3	0.89	6.8	42.1	12.0	0.36
4	38.1	0.93	7.0	41.5	12.6	0.36
5	38.4	0.48	10.3	40.6	10.3	0.50
6	38.3	0.48	10.7	40.9	9.7	0.53
7	38.5	0.74	8.8	41.4	10.6	0.45
8	38.2	0.71	9.4	41.4	10.2	0.48

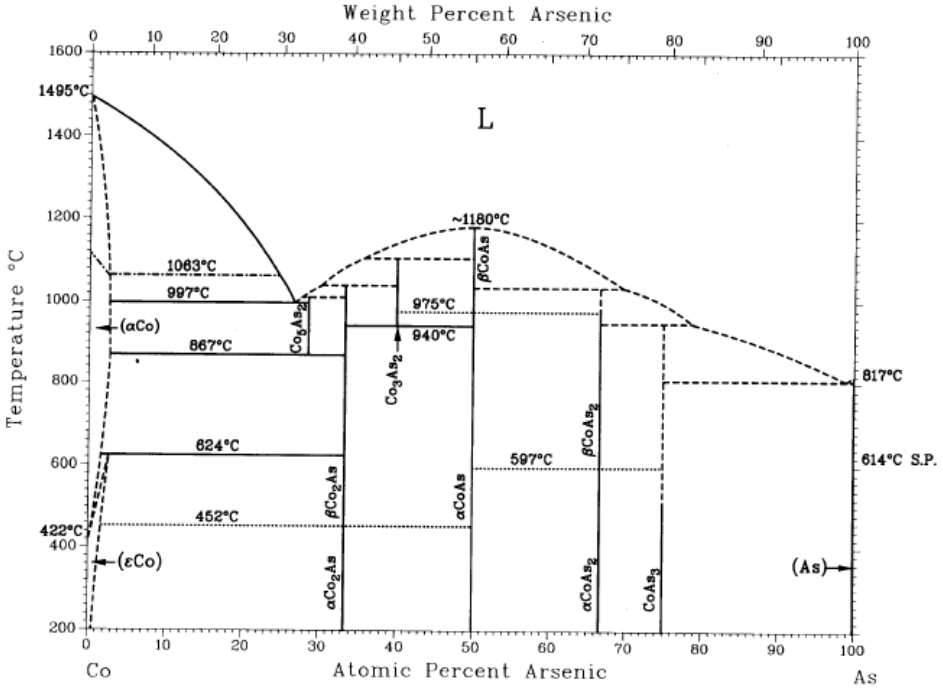
NOTE: from elemental analysis K values vary from plane to plane 40% with 7% std dev.

$BaFe_2As_2$

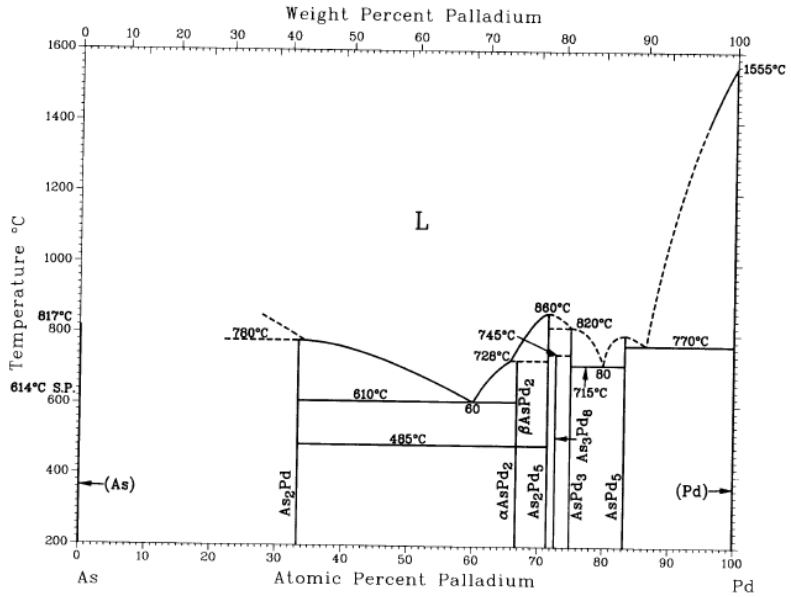
$BaFe_2As_2$ (as well as Sr- and Ca-variants) can be grown out of a FeAs rich melt. In this case the starting melt is based on the binary compound FeAs. This also keeps the vapor pressure down and prevents explosions. Crystals are not so well faceted, but up to multi-grams in mass…..





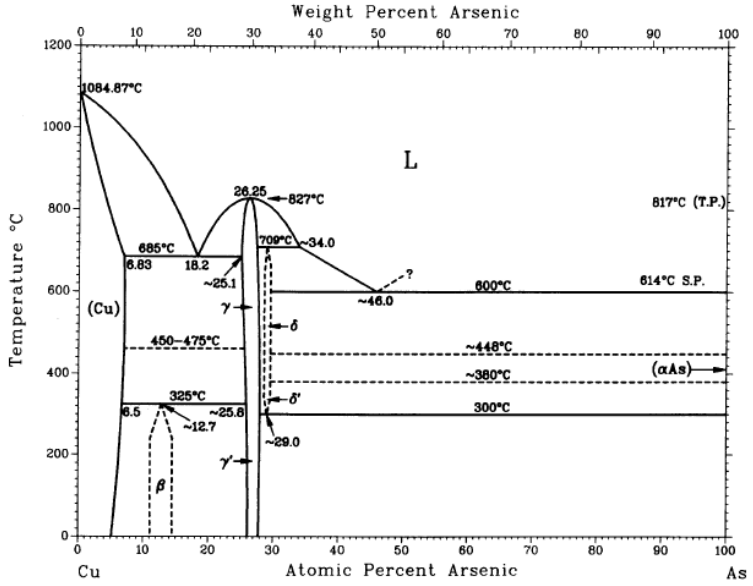


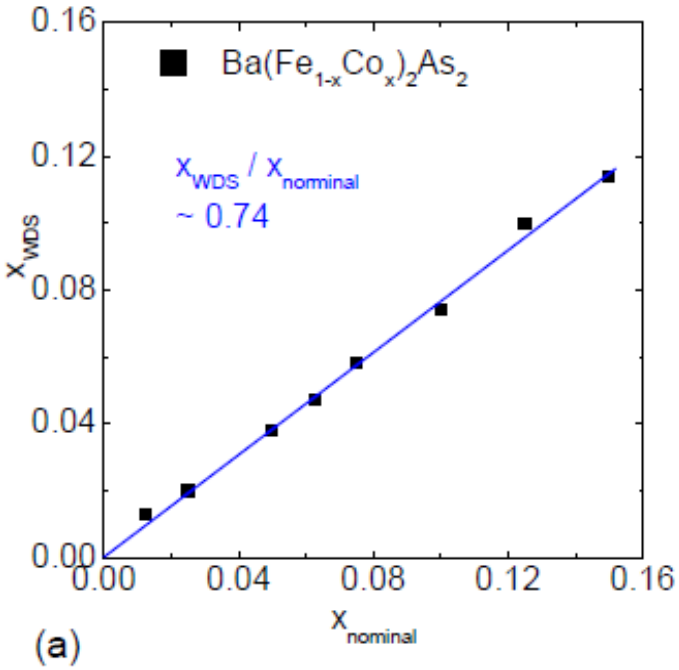
By shifting from one transition metal to another we change the solvent....

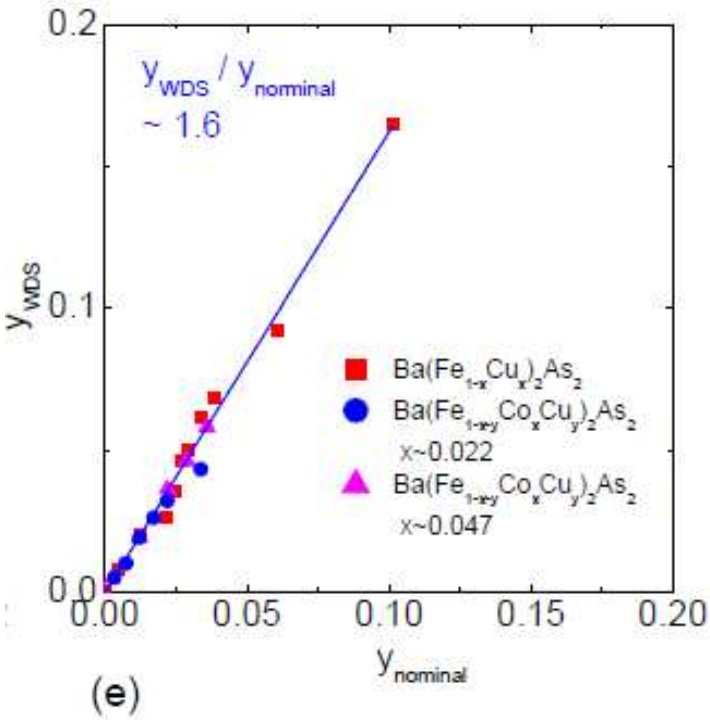


As can be seen these phase diagrams are quite different in detail.

Key detail

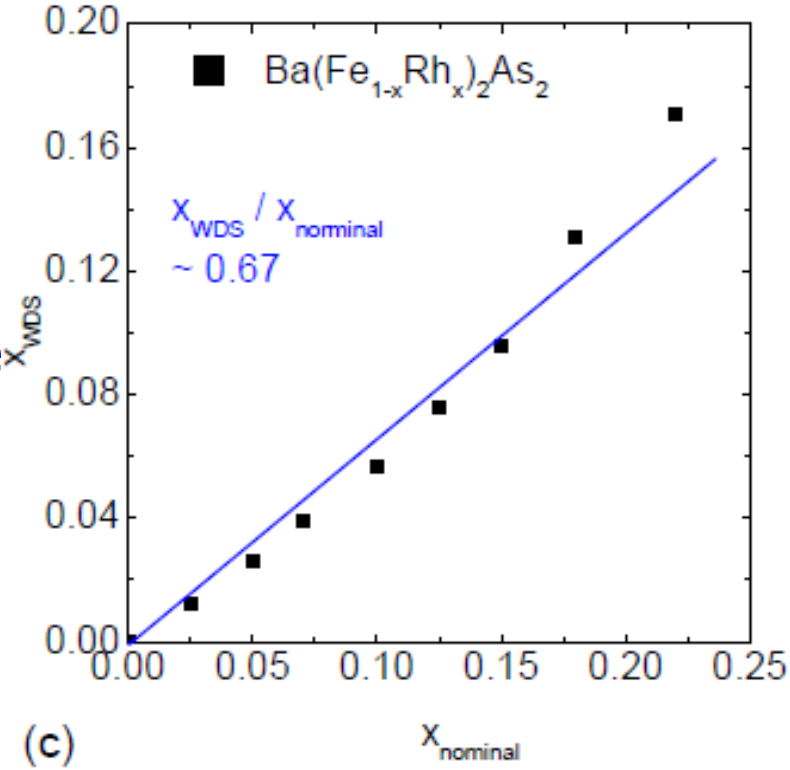


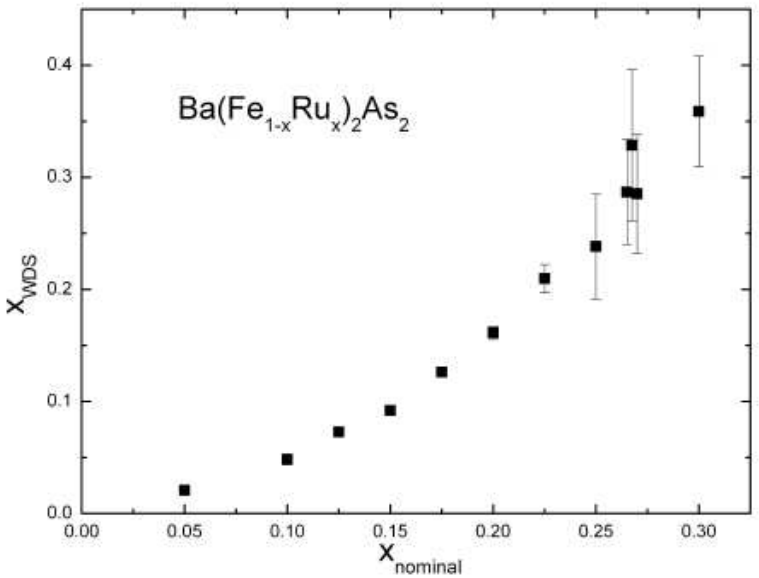




We have used elemental analysis (WDS) to determine the composition of each batch used and also determined the variation within a single sample as well as within a given batch.

This is vital for any quantitative statements or analysis.





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

N	8	8	7	9	7	6	10	5	5	9
$x_{nominal}$	0.0125	0.025	0.05	0.0625	0.075	0.1	0.125	0.15	0.17	0.20
x_{WDS}	0.013	0.02	0.038	0.047	0.058	0.074	0.10	0.114	0.135	0.166
2σ	0.001	0.001	0.002	0.002	0.002	0.003	0.002	0.004	0.002	0.003

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

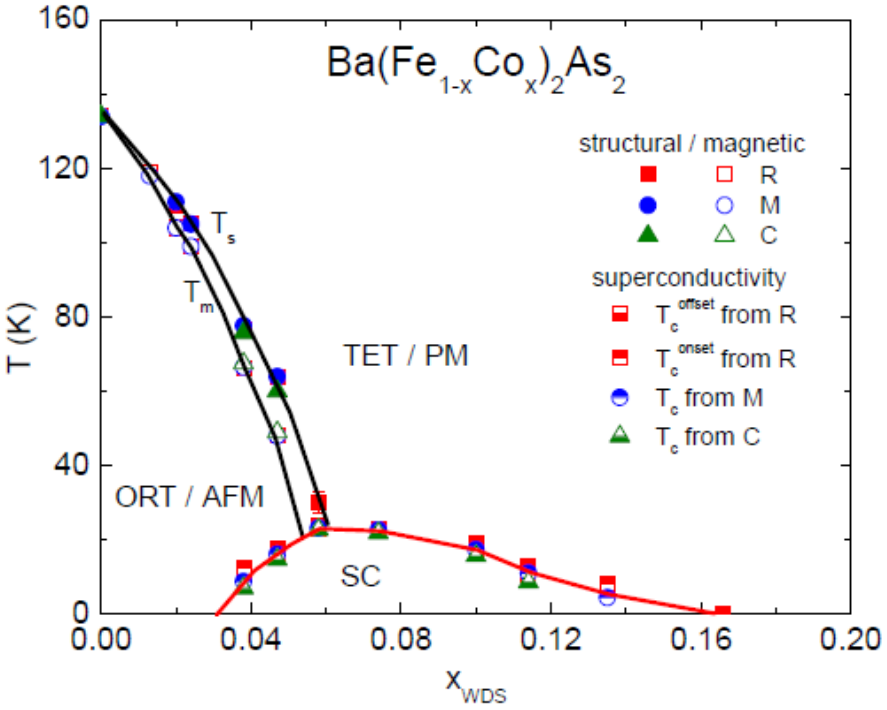
N	18	10	44	18	11	12	28
$x_{nominal}$	0.01	0.02	0.03	0.04	0.05	0.07	0.09
x_{WDS}	0.0067	0.016	0.024	0.032	0.046	0.054	0.072
2σ	0.001	0.002	0.002	0.003	0.002	0.002	0.004

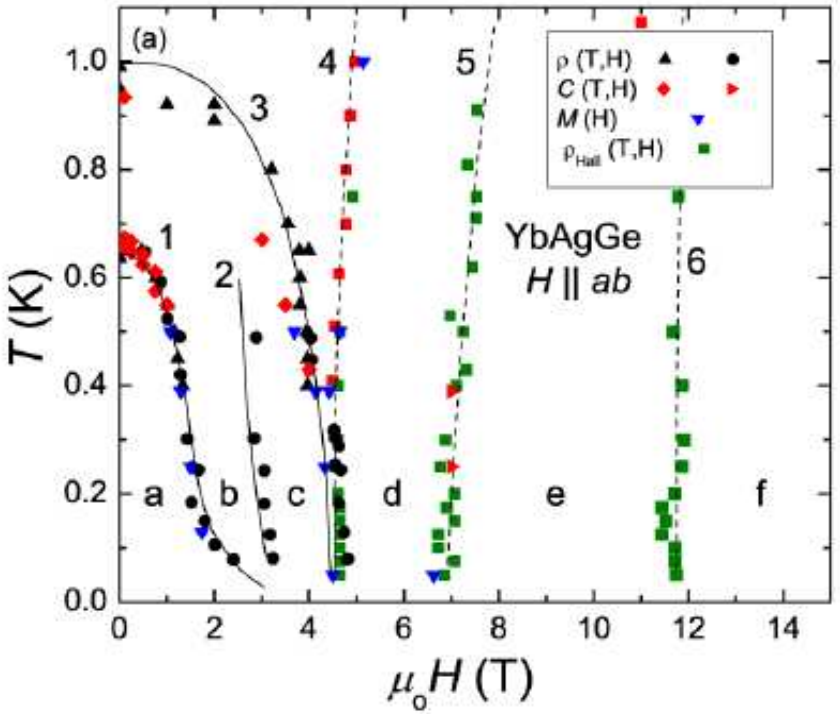
$Ba(Fe_{1-x}Rh_x)_2As_2$

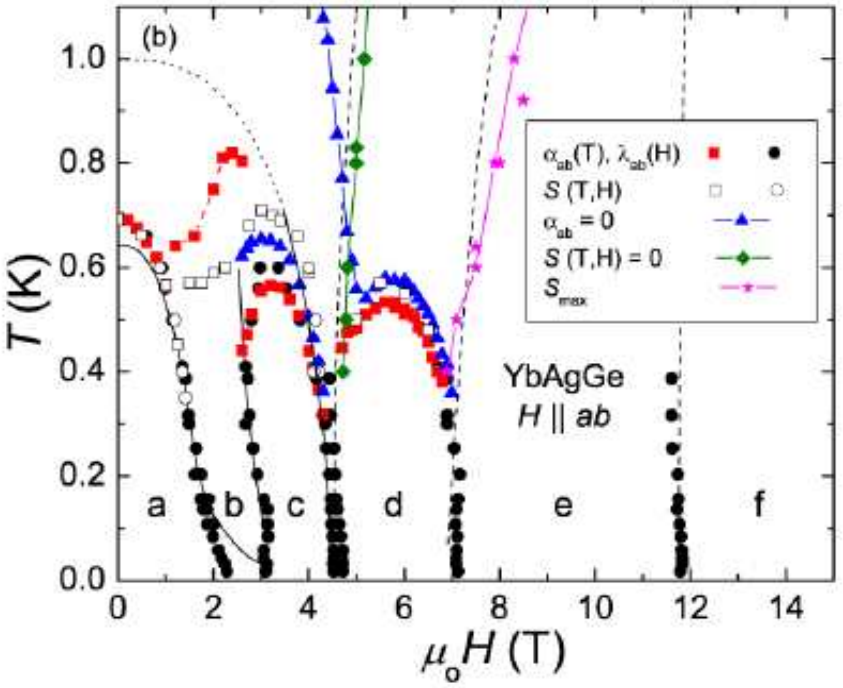
N	16	16	18	15	20	34	33	20
$x_{nominal}$	0.025	0.05	0.07	0.1	0.125	0.15	0.18	0.22
x_{WDS}	0.012	0.026	0.039	0.057	0.076	0.096	0.131	0.171
2σ	0.001	0.001	0.002	0.003	0.004	0.006	0.005	0.002

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

N	18	8	52	6	6	12	14	52
$x_{nominal}$	0.0125	0.025	0.0325	0.04	0.05	0.0625	0.085	0.1
x_{WDS}	0.012	0.021	0.027	0.030	0.043	0.053	0.067	0.077
2σ	0.001	0.002	0.003	0.002	0.001	0.002	0.002	0.005







A lot of information can be place into, and extracted from, phase diagrams.

Constructing them is often difficult and the more experimental methods that provide consistent information the more likely they are to be accurate / reliable.

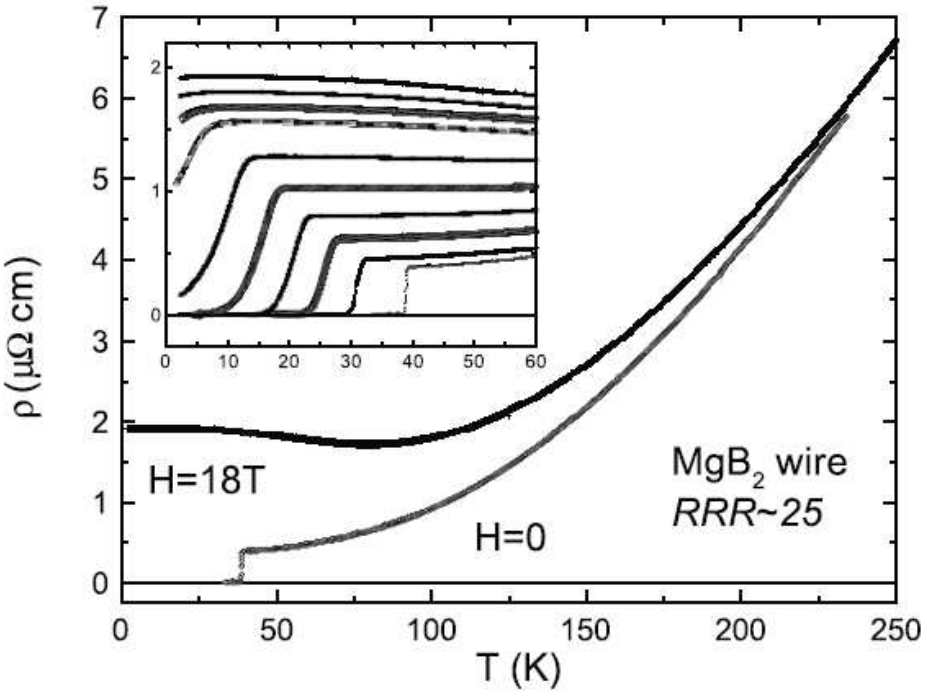
Let's review a few examples….

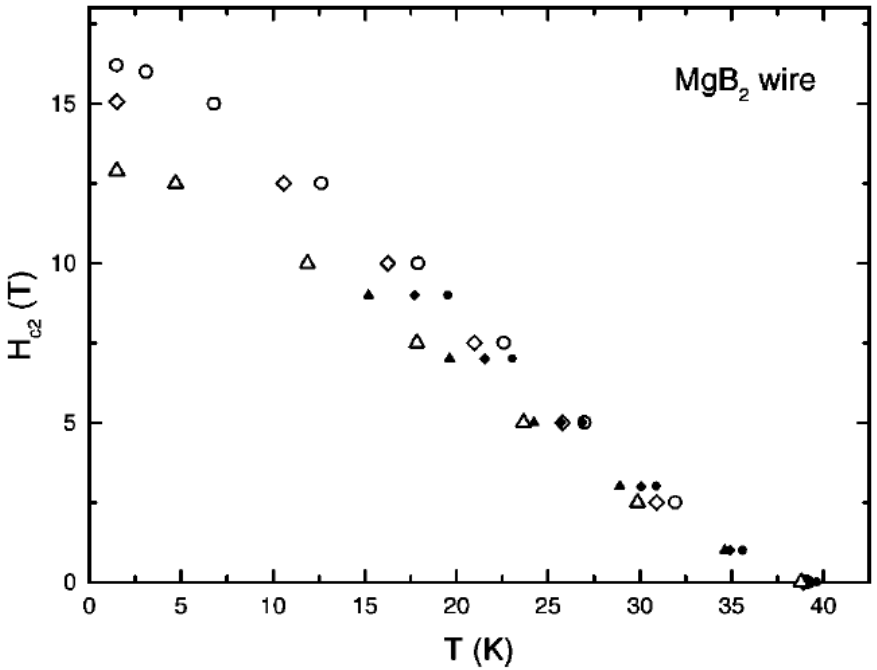
Resistivity / Resistance

Resistivity measurements can be used to learn about the superconducting state, for example in MgB_2.

$\rho(T,H)$ data can be used to delineate the superconducting / normal phase boundary: $H_{c2}(T)$.

But even here, for a *"simple superconductor",* it is important to clearly state the criterion or criteria used to determine a transition point. In this case we illustrated the effect of using an onset, mid-point, and off-set criterion.





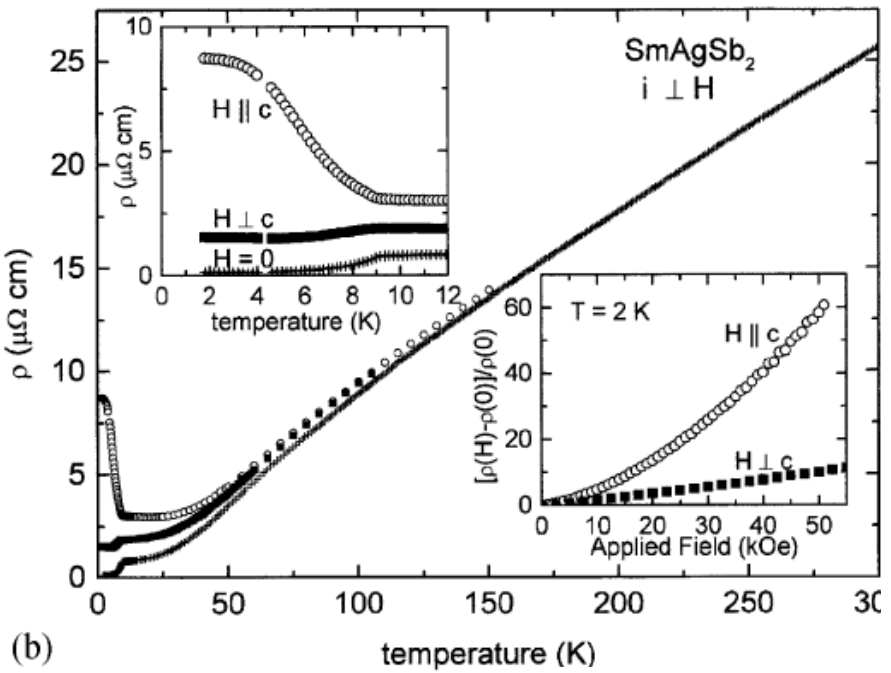
S. L. BUD'KO *et al.* PHYSICAL REVIEW B **63** 220503(R) 2001

Resistivity / Resistance

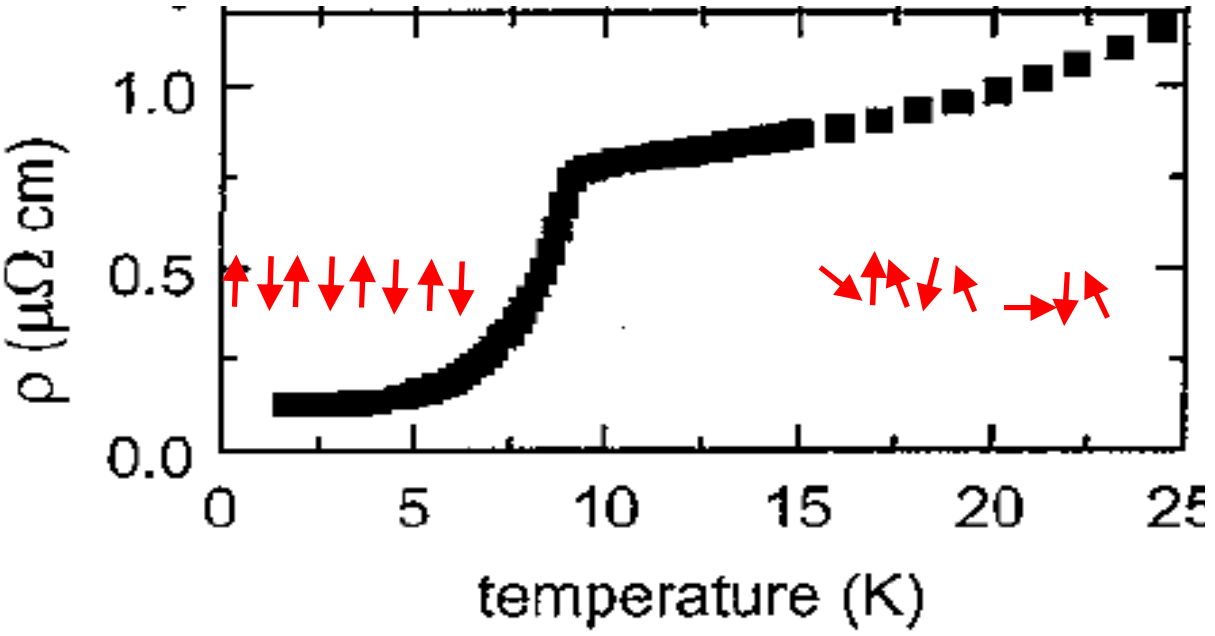
Effects of local moments

ρ_0 decreases with increased order. Structurally this means less defects. The conduction electrons can also couple to localized magnetic moments, such as on rare earths.

When the moments change from disordered (paramagnetic) to ordered (ferromagnetic, antiferromagnetic, or more complex order) there is a decrease in scattering. This is called a loss of spin-disorder scattering.



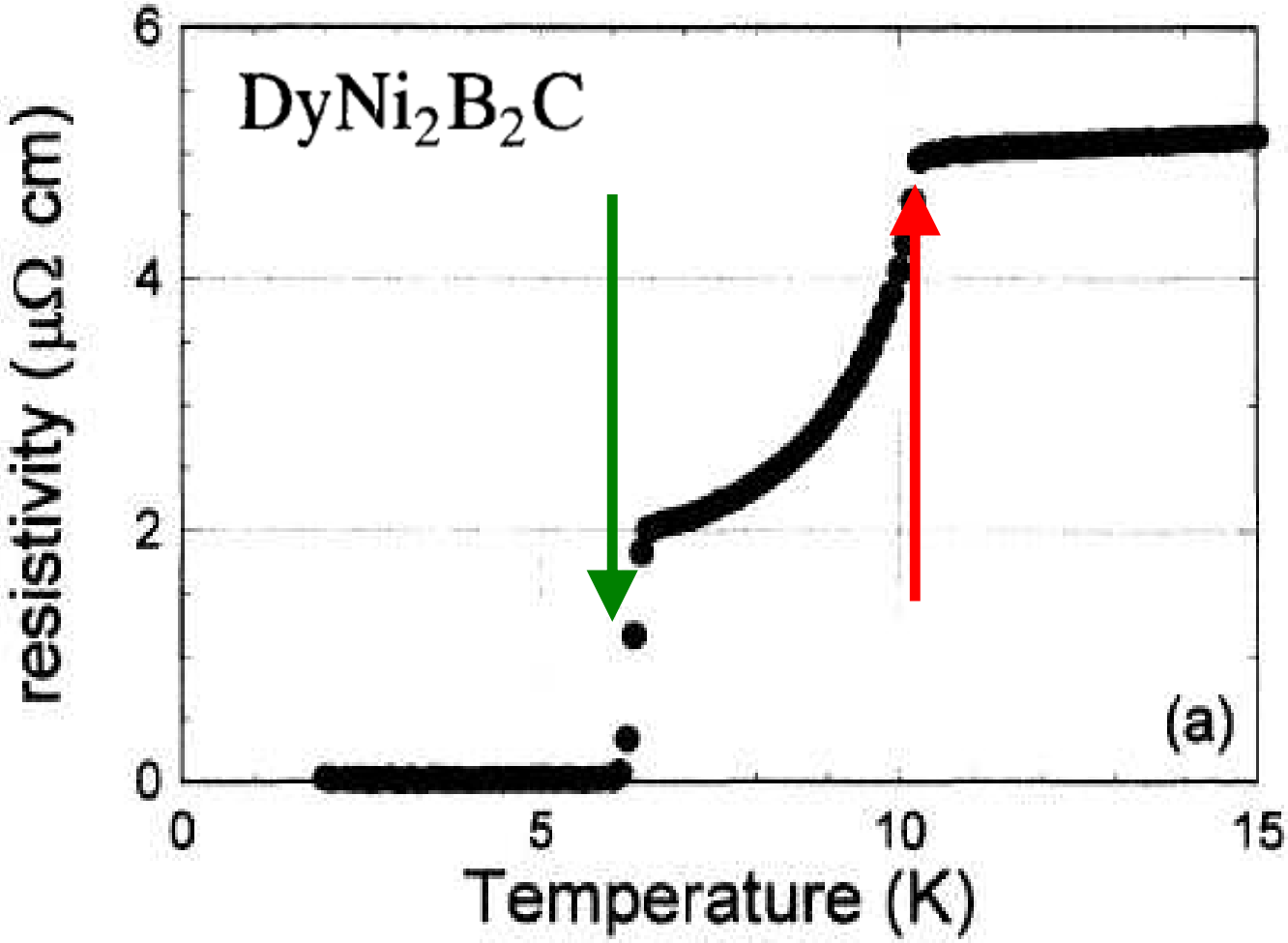
RRR ≈ 200



Journal of Magnetism and Magnetic Materials 205 (1999) 27–52

Resistivity / Resistance

Multiple transitions can be easily detected and identified: In this case we have a rare example of T_N ~ 10 K with the loss of spin disorder scattering, followed at lower temperatures by T_c ~ 6K and a total loss of resistivity.



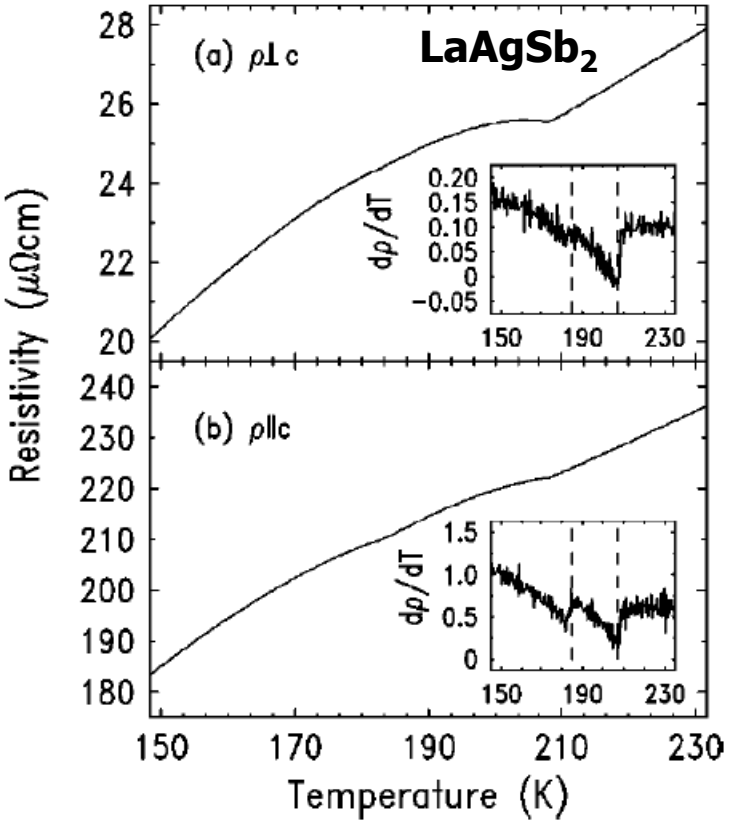
B. K. Cho, P. C. Canfield, and D. C. Johnston PHYSICAL REVIEW B 52 R3844 1 AUGUST 1995-II

Resistivity / Resistance --- Density waves

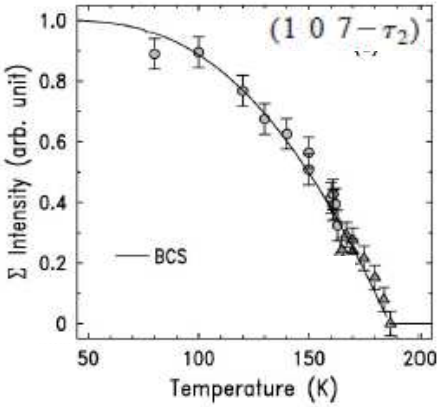
Resistivity is also very sensitive to changes in the Fermi Surface:

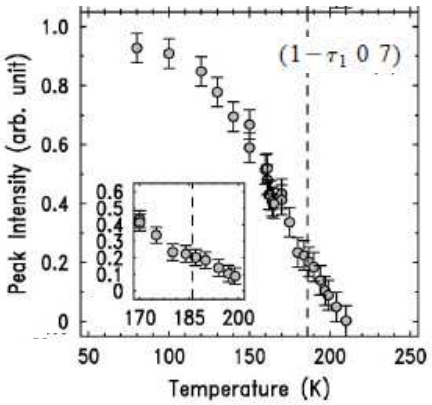
Kubo formula: $\sigma = (1/4\pi^3)(e^2/3\hbar)\int \Lambda dS_F$

This can be seen in CDW (and SDW) transitions, where nested parts of the Fermi surface become gapped below T_{CDW}. This leads to an decrease in σ due to a decrease S_F. For a partial gapping of the F.S. the sample remains metallic and ultimately returns to $\rho(T)$ with positive slope.



NOTE: We thought we saw something curious in the c-axis $\rho(T)$ data….We needed scattering data to confirm the fact that there were indeed two CDW transitions at 207 and 185 K.



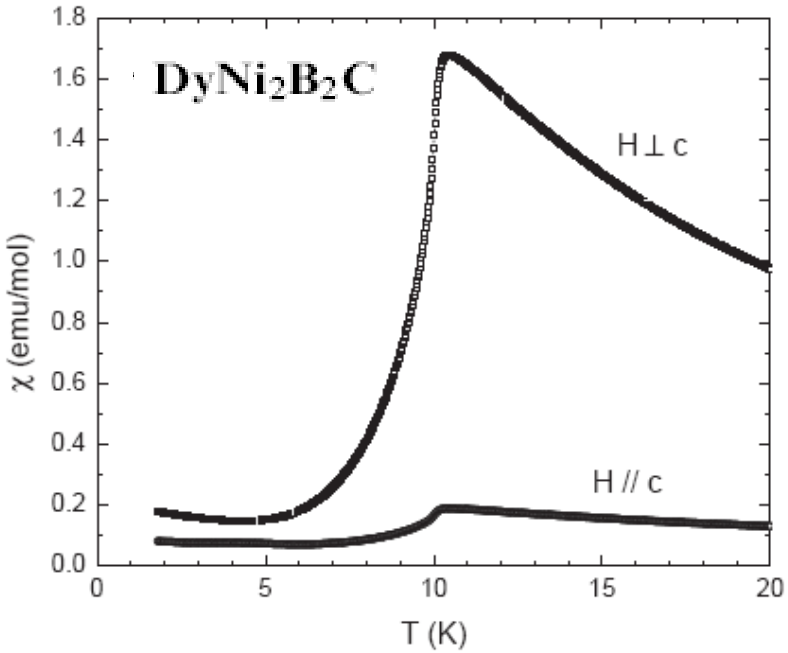


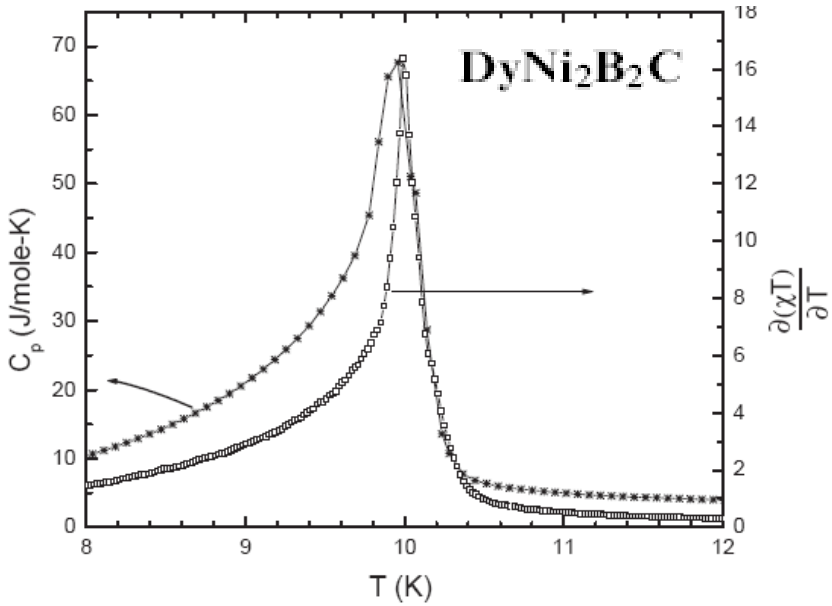
K.D. Myers et al. / Journal of Magnetism and Magnetic Materials 205 (1999) 27–52

C. SONG et al. PHYSICAL REVIEW B 68, 035113 (2003)

Magnetic susceptibility

In addition allowing for evaluation of p_{eff} and θ the magnetic susceptibility can be used to determine the antiferromagnetic ordering temperature, T_N. Although it is tempting to simply take the temperature of the maximum χ value, this only gives a rough estimate. Near T_N, $d(\chi T)/dT$ has the same temperature dependence as C_p,* so the temperature of the maximum in $d(\chi T)/dT$ is considered a more reliable criterion for determination of T_N.





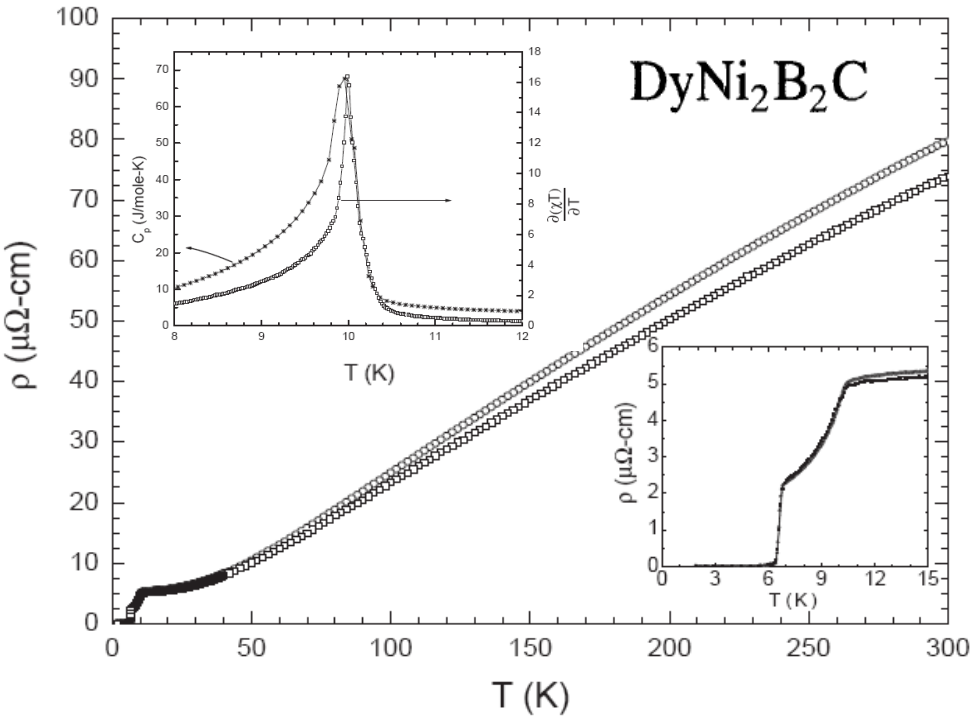
*M. Fisher, Philos. Mag. 7 (1962) 1731.

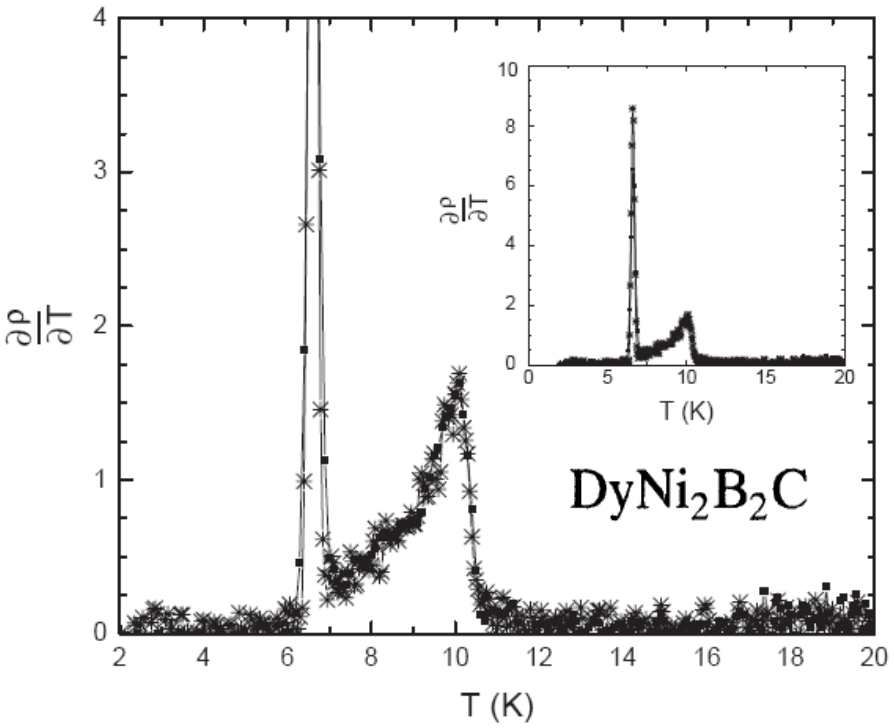
R.A. Ribeiro et al. / Journal of Magnetism and Magnetic Materials 267 (2003) 216–223

A detour back to resistivity for a moment

dρ/dT can also show similar temperature dependencies near T_N,* but only for a limited number of transitions. In general though, dρ/dT can be used as a criterion for T_N or T_C, but this will depend on the noise level of the data.

* M. E. Fisher, J. S. Langer, Philos. Mag., 7 (1962) 1731.

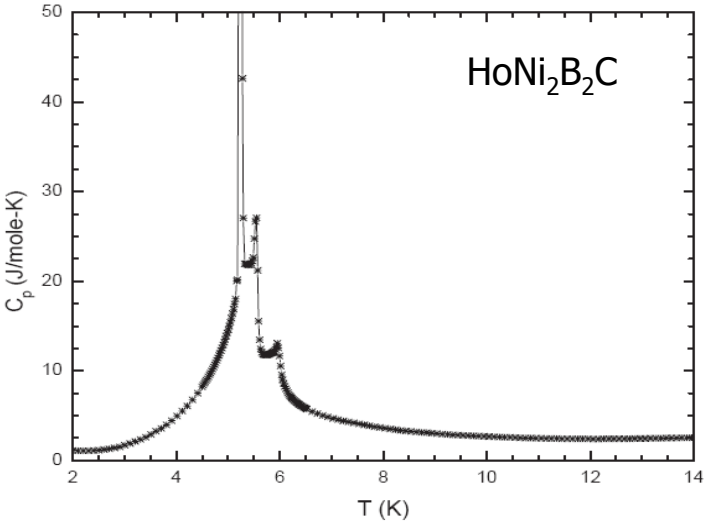


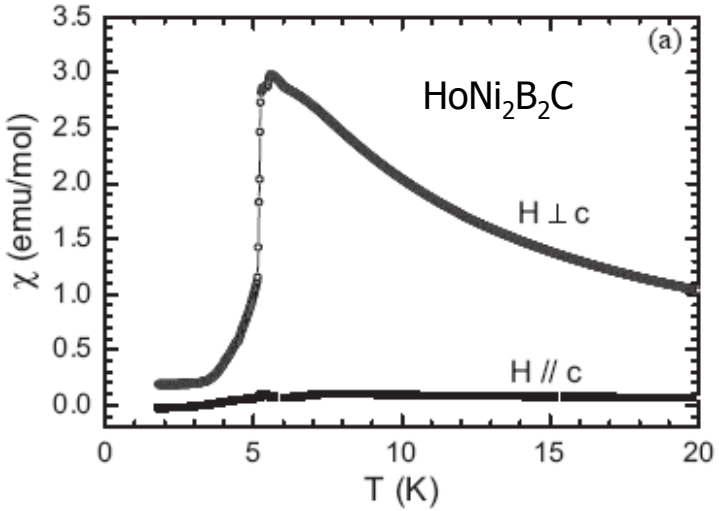


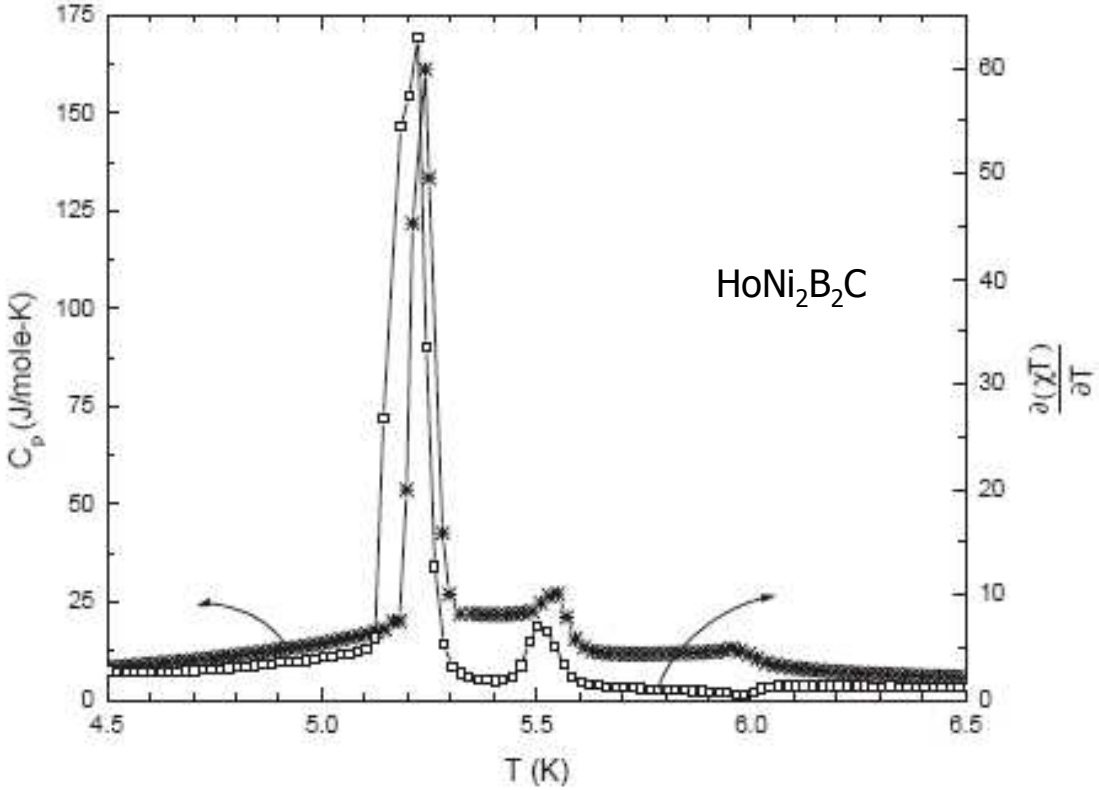
R.A. Ribeiro et al. / Journal of Magnetism and Magnetic Materials 267 (2003) 216–223

Multiple transition temperatures

$HoNi_2B_2C$ has a cascade of magnetic transitions (AF) between 6 and 5 K. They are clear in both C_p and χ data.







Although it lacks formal, theoretical under-pinning, it is reasonable, and empirically justified to again use $d\chi T/dT$ to locate transition temperature in $\chi(T)$ data.

P. C. Canfield et al. / Physica C (1994), 230(3-4), 397-406 AND

R.A. Ribeiro et al. / Journal of Magnetism and Magnetic Materials 267 (2003) 216–223

Back to the FeAs system

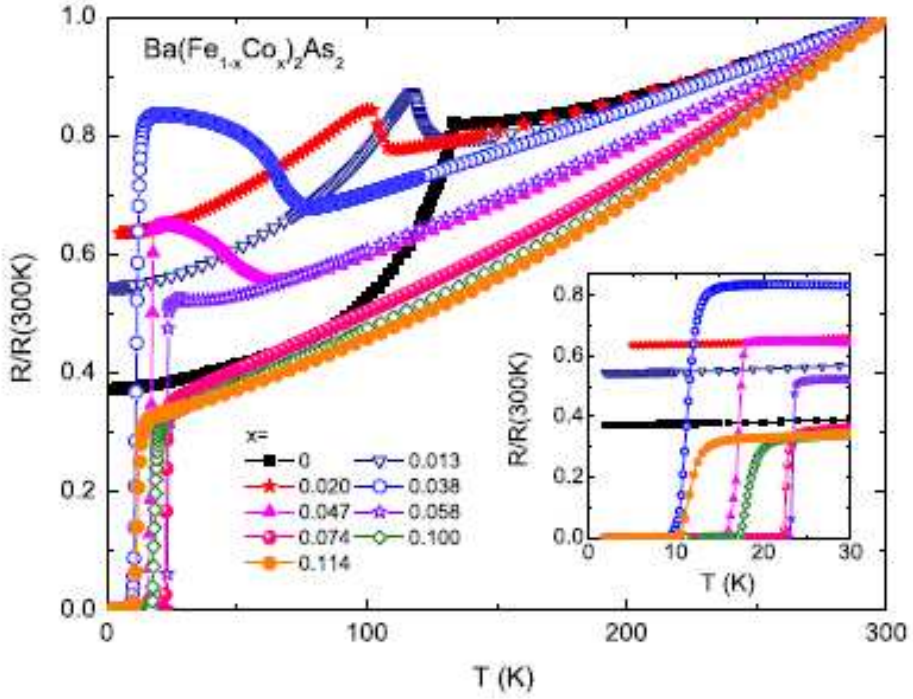
For Co-doped $BaFe_2As_2$ there was a clear suppression of the signature of the combined structural / magnetic phase transition with Co addition. On the other hand, this was not a trivial transition and as it was suppressed it seemed to either broaden or split…..

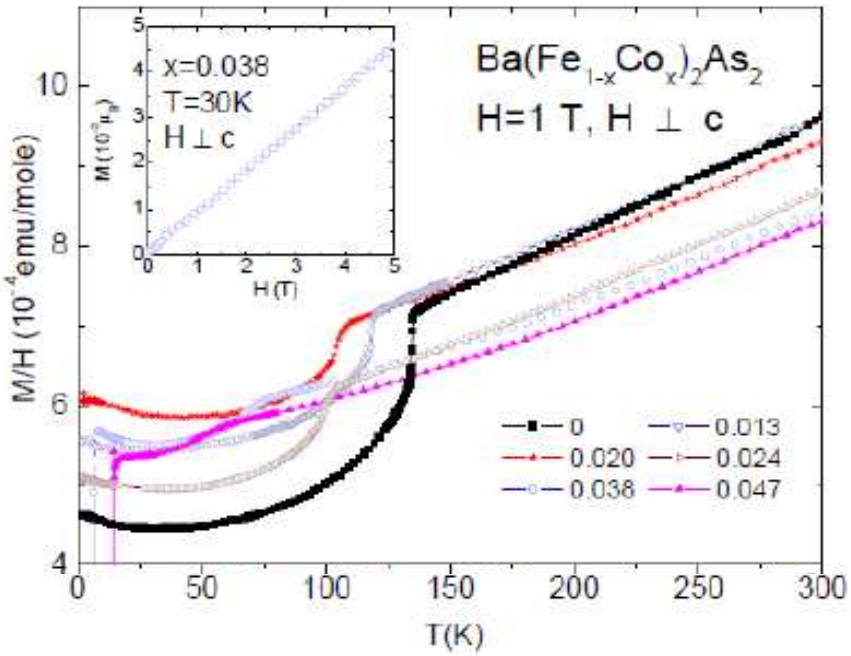
PHYSICAL REVIEW B 78, 214515 (2008)

Effects of Co substitution on thermodynamic and transport properties and anisotropic H_{c2} in $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals

N. Ni,[1] M. E. Tillman,[1] J.-Q. Yan,[1] A. Kracher,[1] S. T. Hannahs,[2] S. L. Bud'ko,[1] and P. C. Canfield[1]

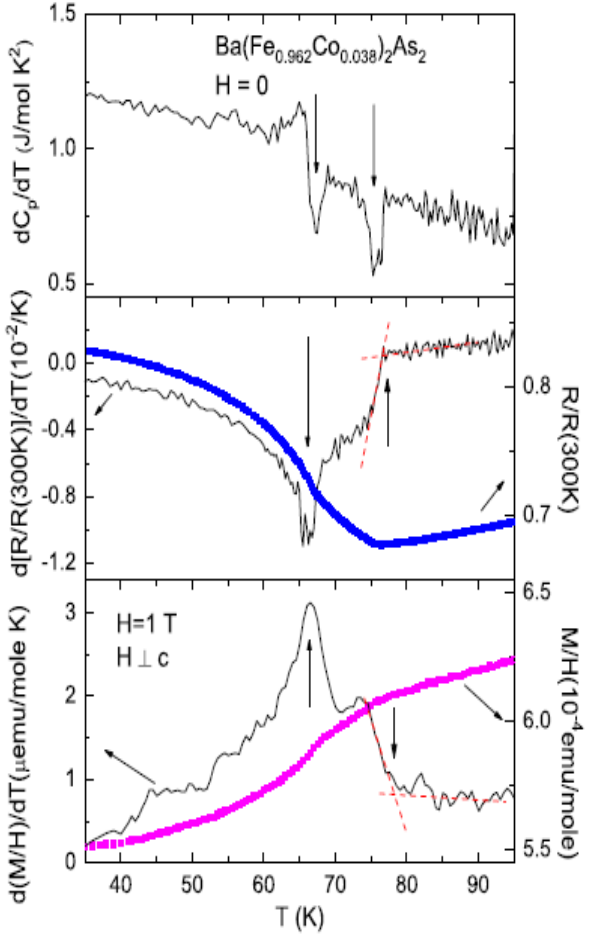
(Received 11 November 2008; published 29 December 2008)

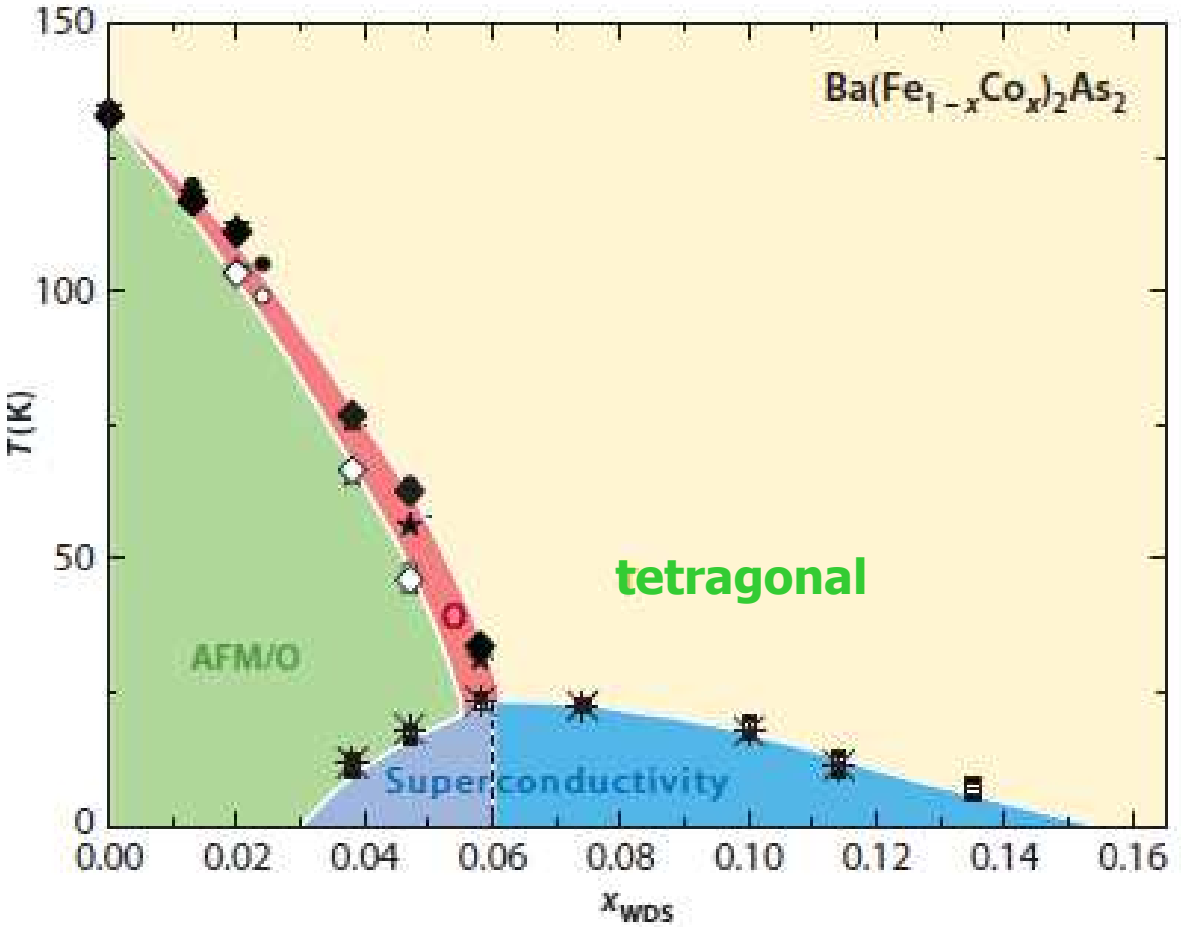




Using thermodynamic and transport data we could assemble a T-x phase diagram that clearly showed (i) superconducting dome existing in both ortho/AF and tetragonal phases and (ii) a splitting (or broadening) of the x = 0 simultaneous orthorhombic and antiferromagnetic phase transition. These results are very robust and have been reproduced by several groups.

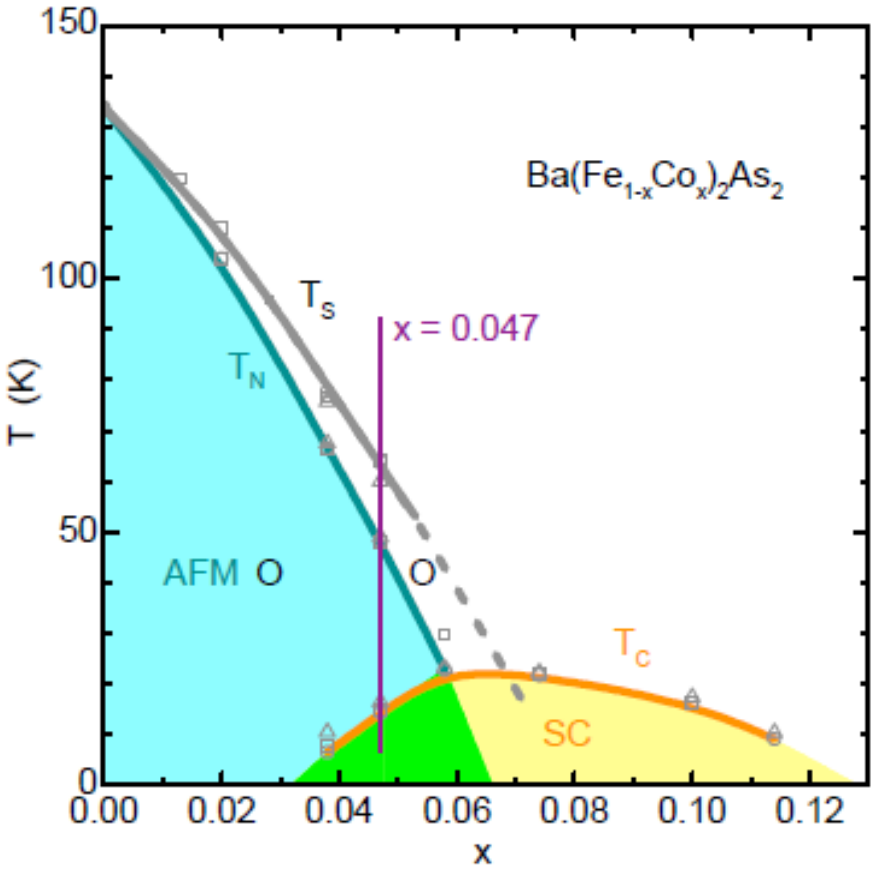
To clarify point (ii) microscopic data was needed….

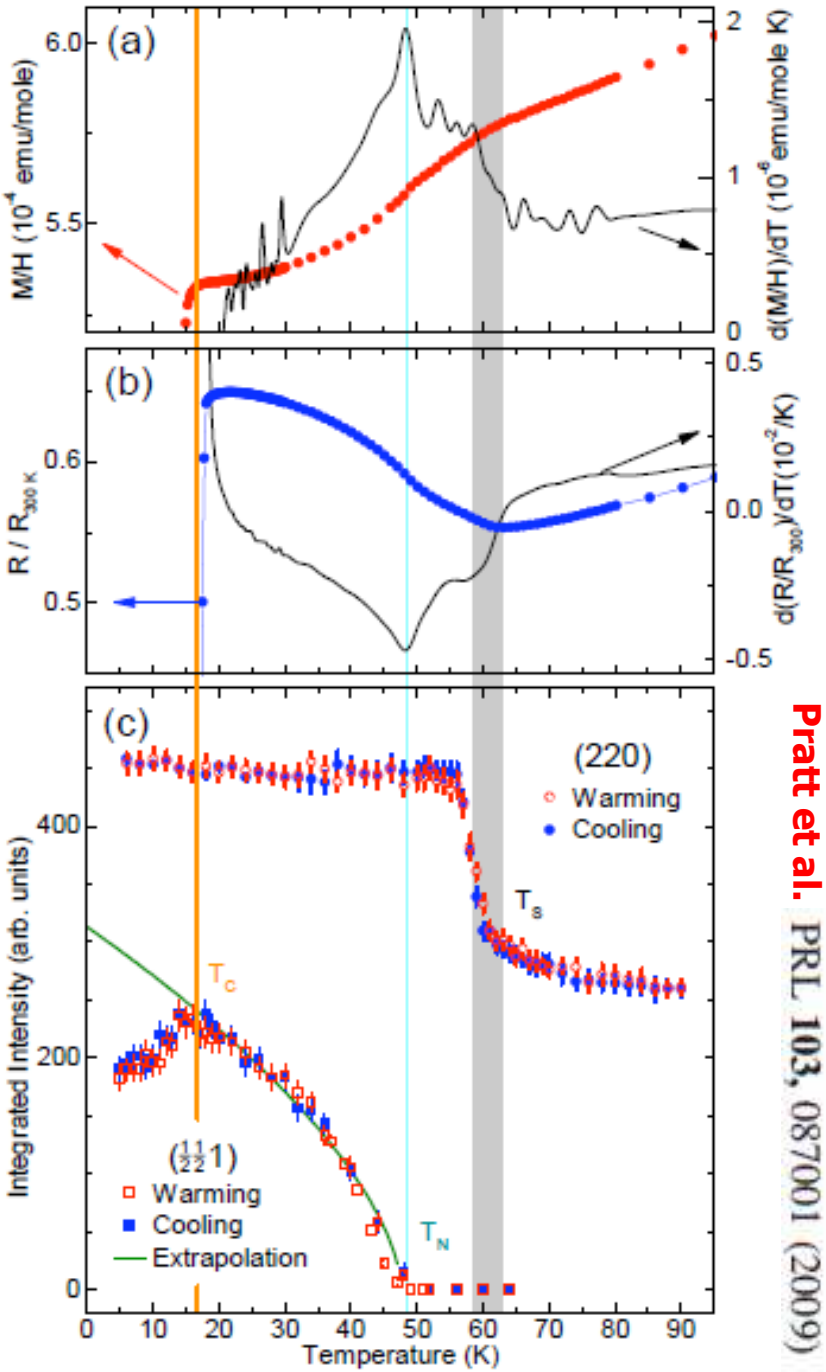




NI *et al.* PHYSICAL REVIEW B 78, 214515 (2008)

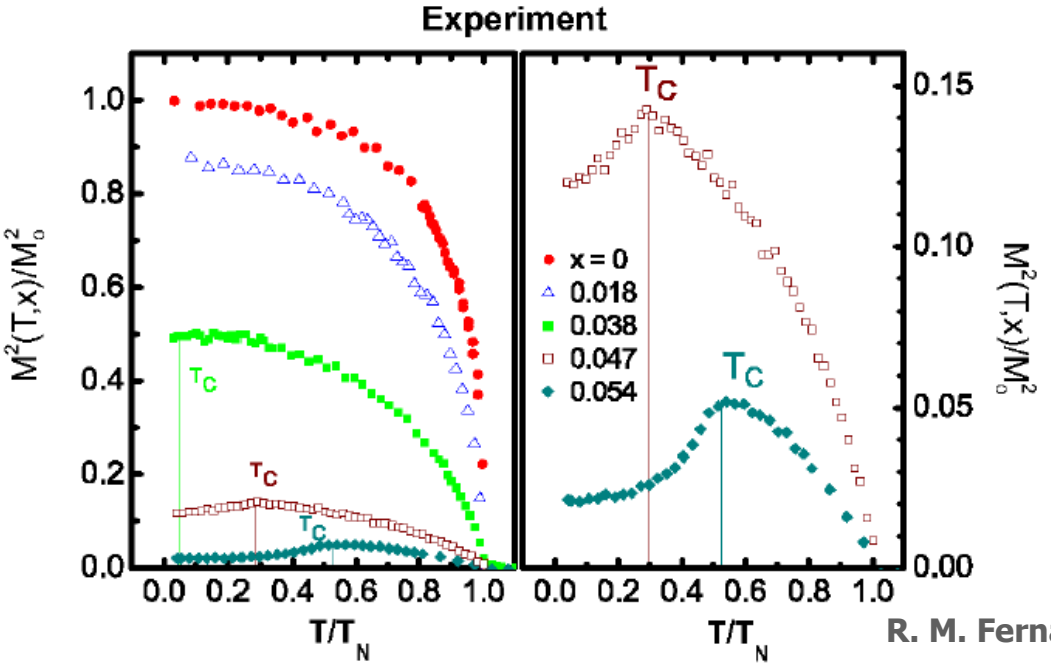
Neutron and X-ray scattering clarified the question of splitting versus broadening. There is a clear separation between the structural (upper transition) and magnetic (lower). This confirms the criterion we used to infer them from our bulk measurements.



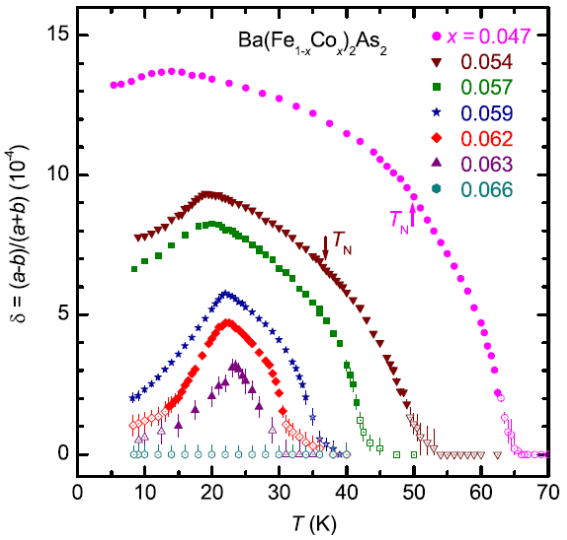


Pratt et al. PRL 103, 087001 (2009)

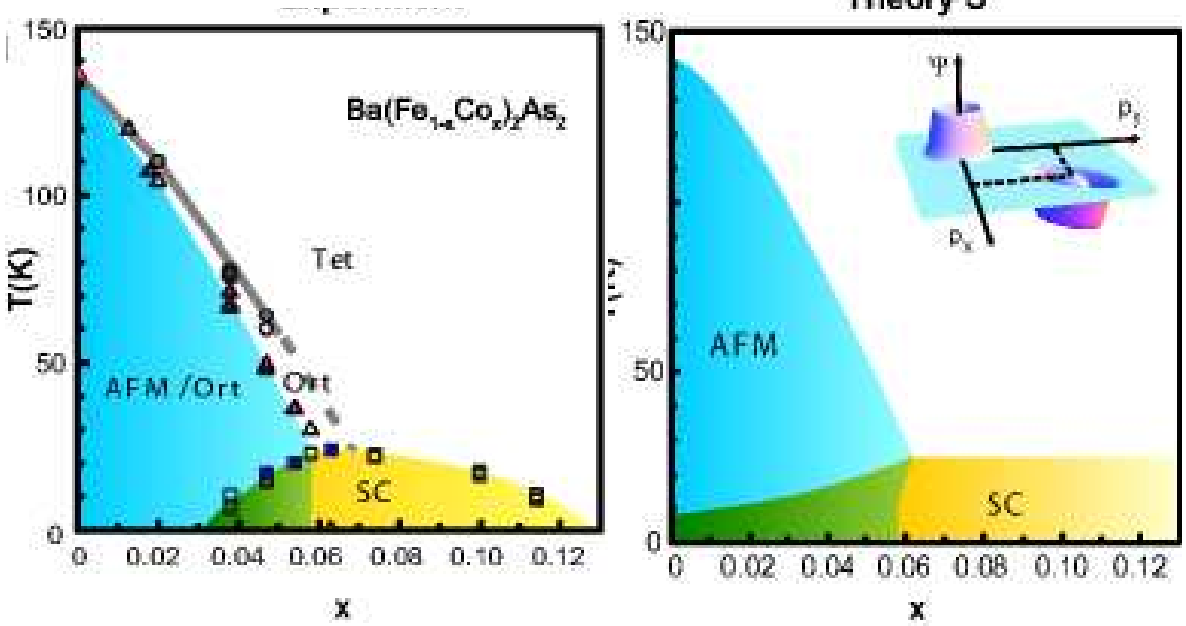
Extensive neutron and X-ray scattering measurements established that both the magnetic order and the higher temperature, ortho-splitting are profoundly effected by, and probably compete with, the superconducting state. Recent theoretical work shows that this is consistent with a S^{+-} pairing in the superconducting state.



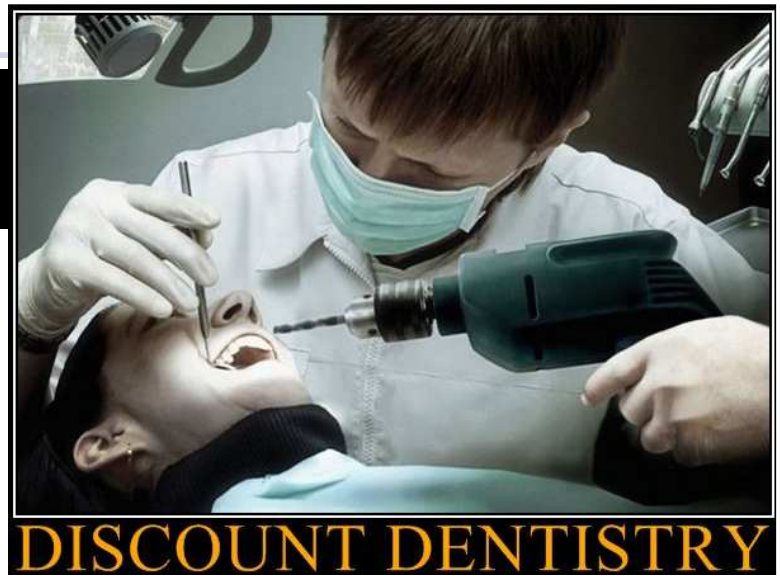
R. M. Fernandes et al. PHYSICAL REVIEW B 81, 140501(R) (2010)



S. Nandi et al. PRL 104, 057006 (2010)



Caveat Emptor!



So, when you are trying to define the phase diagrams of new materials, with potentially new physics, you need to be:

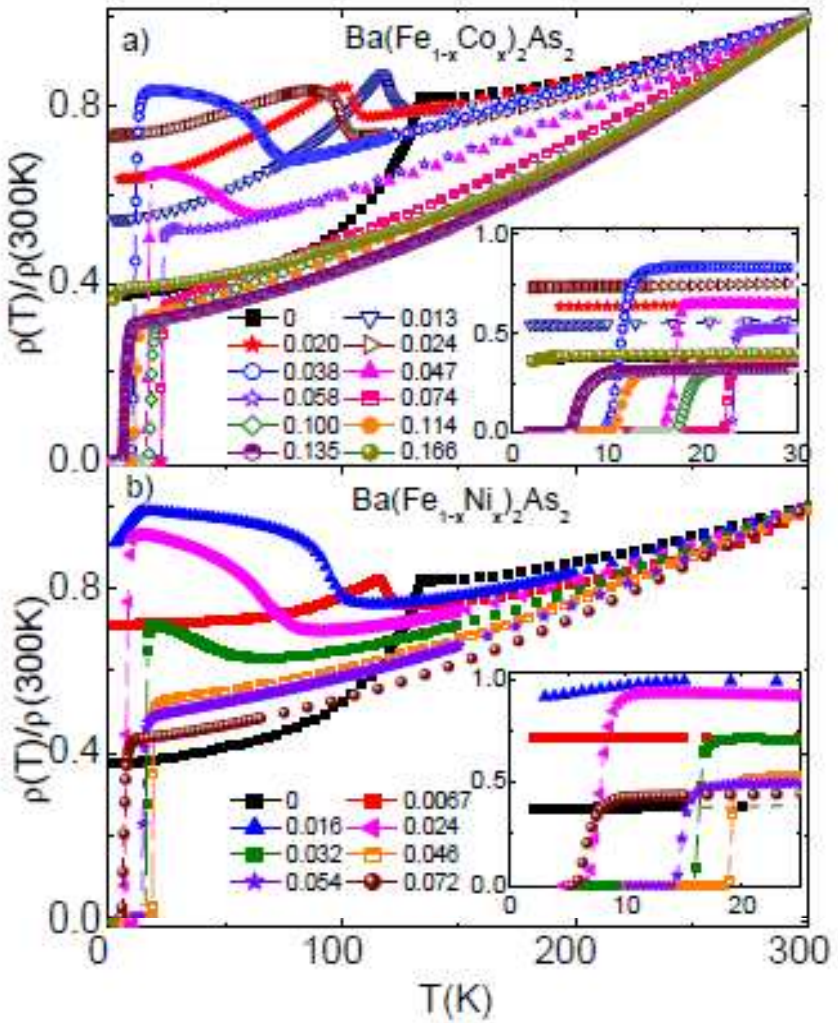
1) Careful to state what your criterion are,
2) Keep in mind that features may be real physics or simply artifacts
3) Do your best to justify claims by performing the needed follow up measurements.

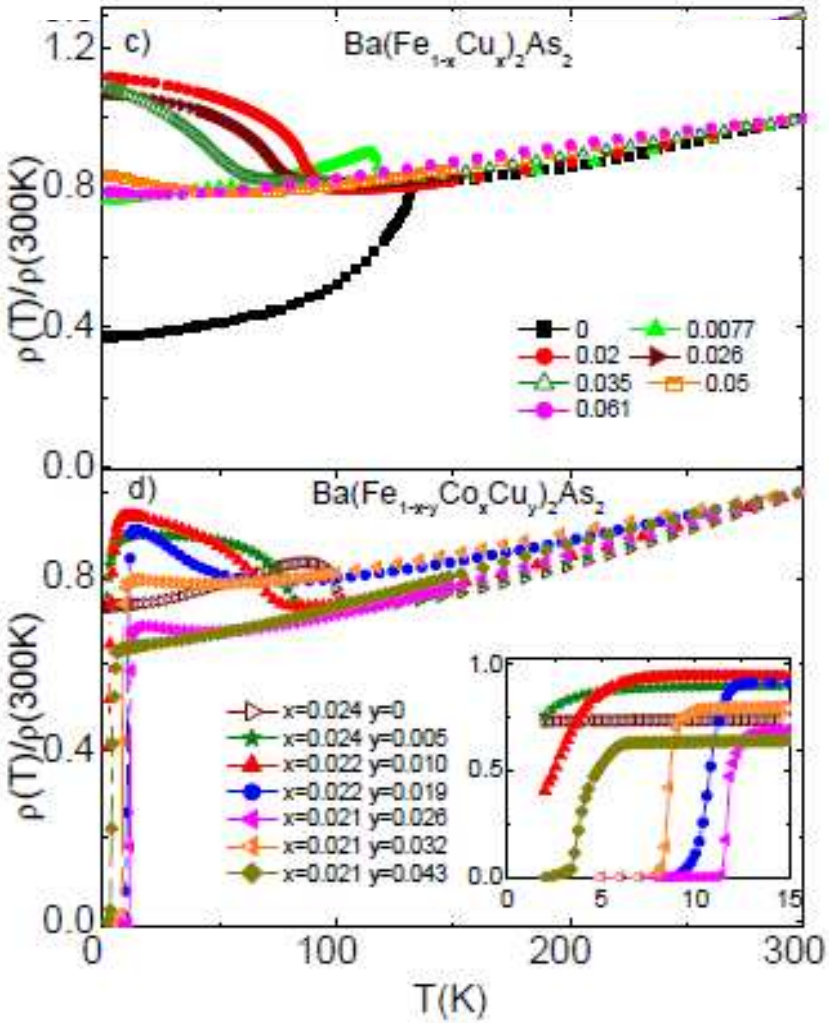
This may all be "common sense" but in the heat of new discovery sometimes researchers will forget the importance of these steps.

In addition, for my theoretical friends, a care must be taken in deciding what data should be taken seriously and what data should be handled with varying degrees of skepticism….Caveat Emptor!!!

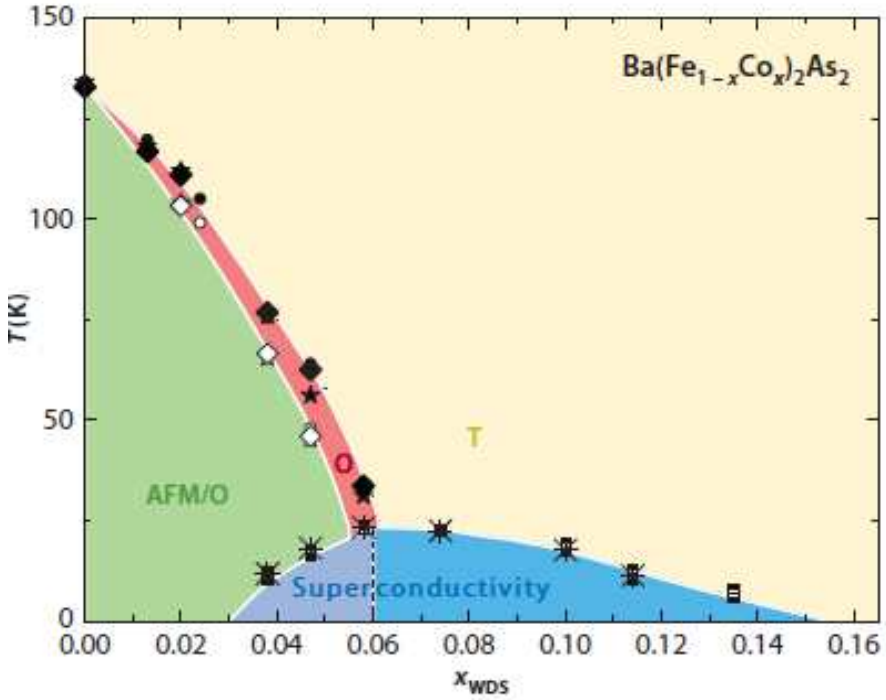
Examine the effects of TM substitution further: TM = Co, Ni, and Cu

Ni- and Cu-doping suppress the upper transitions in a manner similar to Co.
Whereas Ni stabilizes superconductivity, Cu does not for T > 2 K.
To prove that Cu-doping was not poisonous to S.C. we examined a Co/Cu doping.

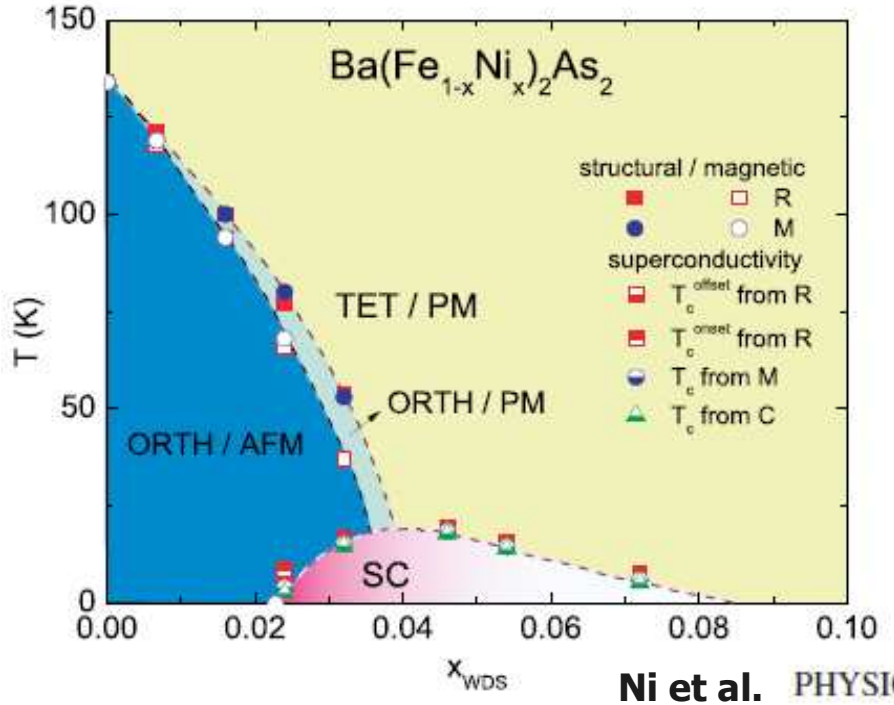


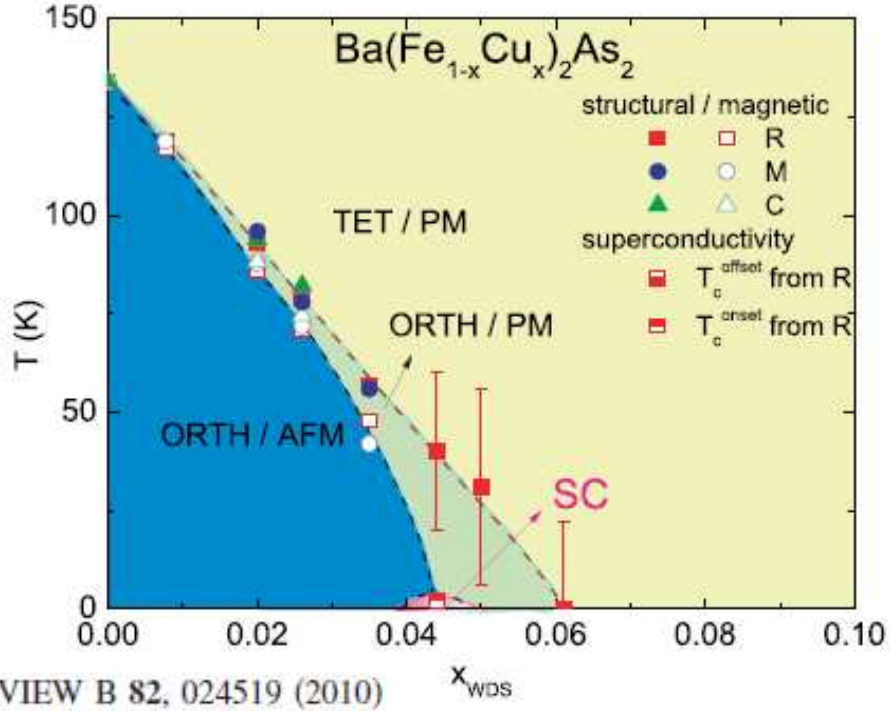


PHYSICAL REVIEW B 80, 060501(R) (2009)



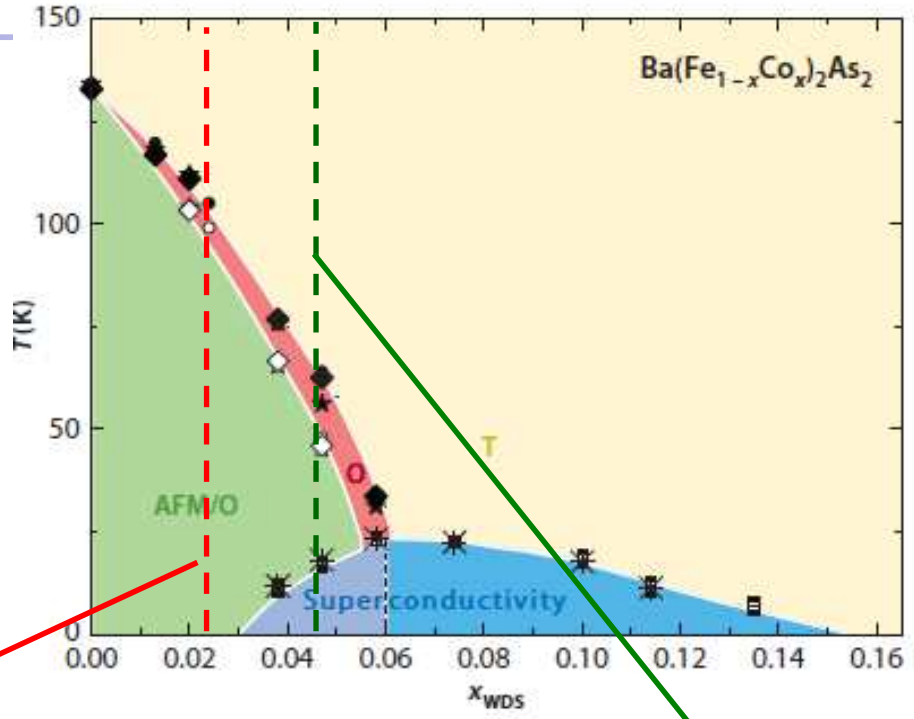
Using resistivity, magnetization, and specific heat measurements, and adding more samples and series too, phase diagrams for 3d-TM doping can be assembled and examined.

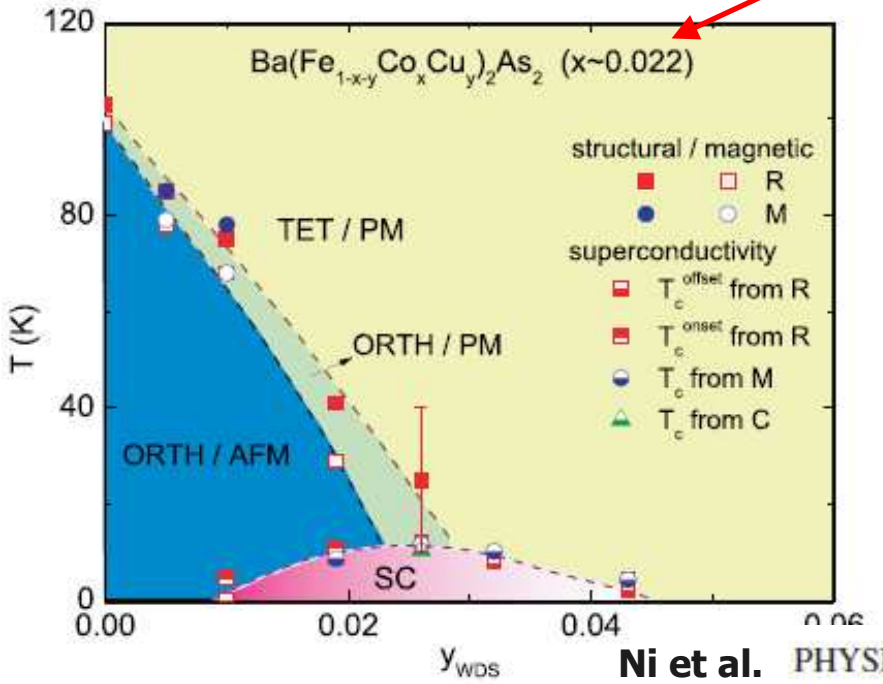


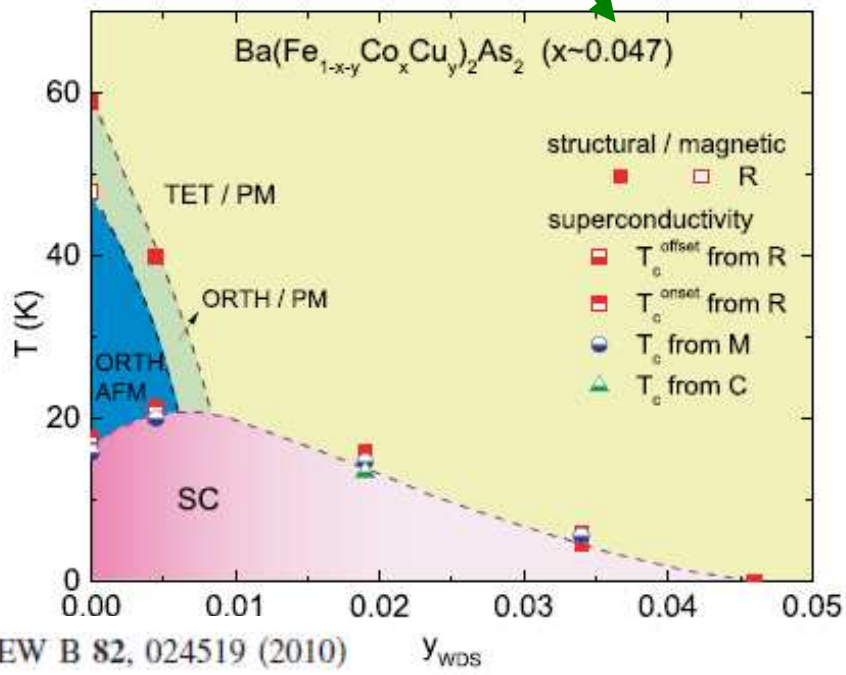


Ni et al. PHYSICAL REVIEW B **82**, 024519 (2010)

Although Cu doping alone barely manages to stabilize superconductivity, Cu itself is not somehow poisonous. Adding Cu to lightly Co-doped $BaFe_2As_2$ allows for the discovery of similar phase diagrams.







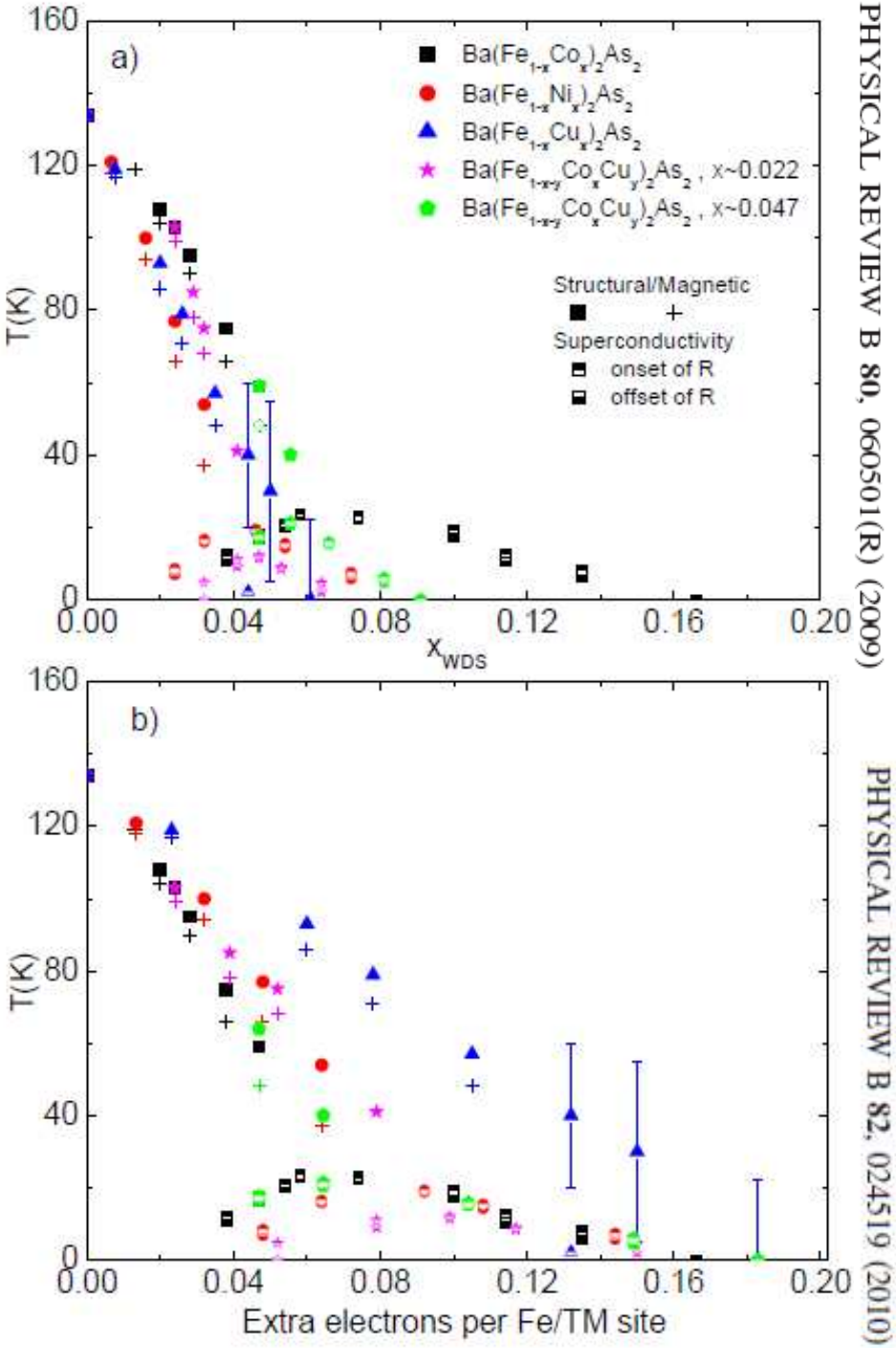
Ni et al. PHYSICAL REVIEW B **82**, 024519 (2010)

By substituting various TM for Fe in $BaFe_2As_2$ we change vary a number of different, but correlated, parameters.

The two most obvious are the number of impurities (x) and the change in electron count (e).

We directly measure x for each sample via WDS and we infer e as follows: for Co --- e = x, for Ni --- e = 2x, for Cu --- e = 3x.

Whereas the upper, structural and magnetic phases transitions scale better with x, the lower, superconducting phase transition scales with e, especially on the overdoped side of the dome.

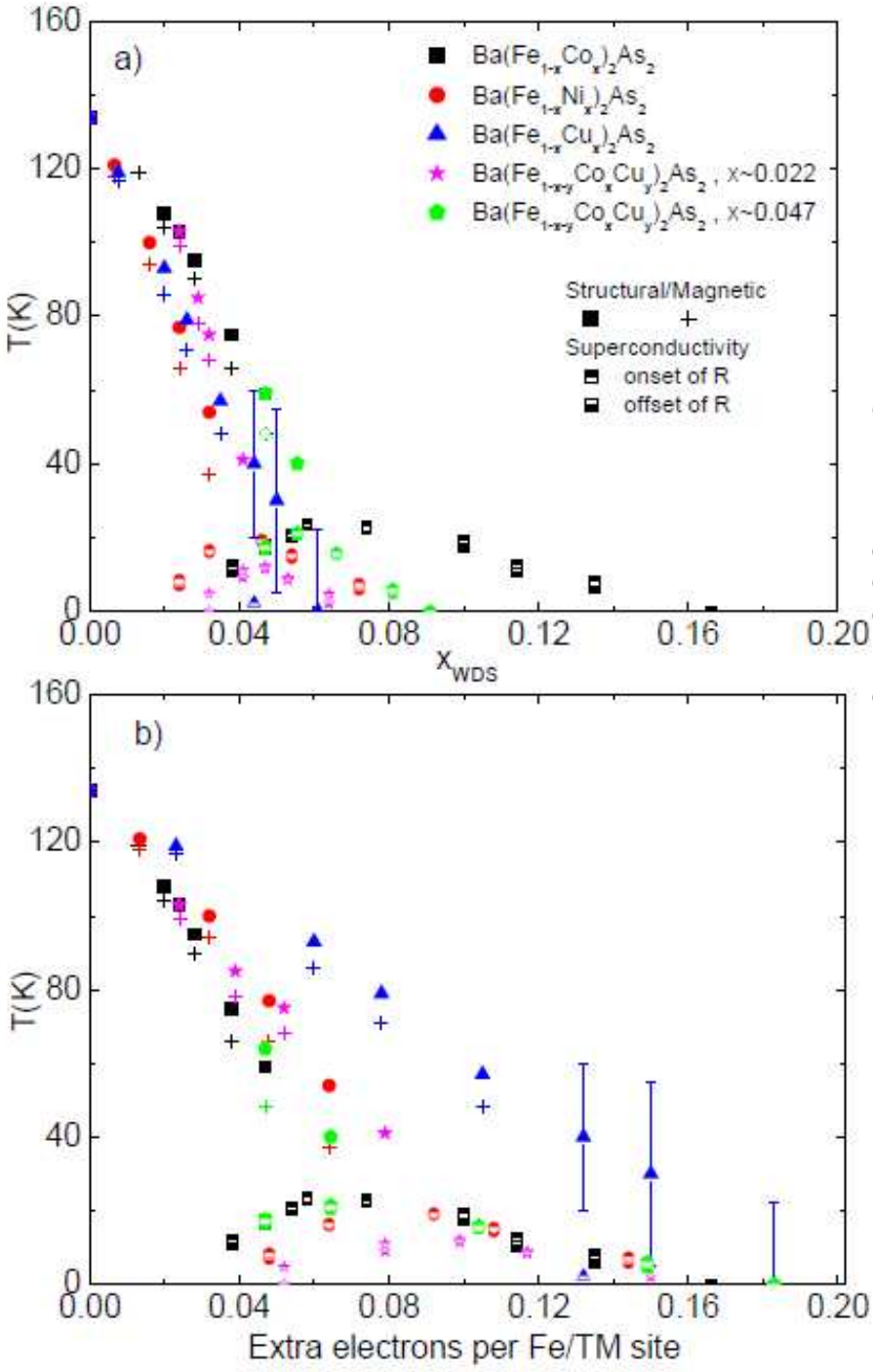


These data show that suppression of the upper, structural / antiferromag transitions is a necessary, but not sufficient condition for superconductivity.

There is a region of e (bandfilling??) that can support superconductivity IF the structural / AF transition ($T_{S/M}$) is suppressed sufficiently.

We can hypothesize that if $T_{S/M}$ is suppressed sufficiently, then the low temperature state is sufficiently similar to the tetragonal state that the superconductivity can be stabilized, even in the ordered state. *(E.g. reduce the size of distortion and / or ordered moment or change fluctution spectrum.)*

This can explain poorer scaling of T_c with e on under doped side.

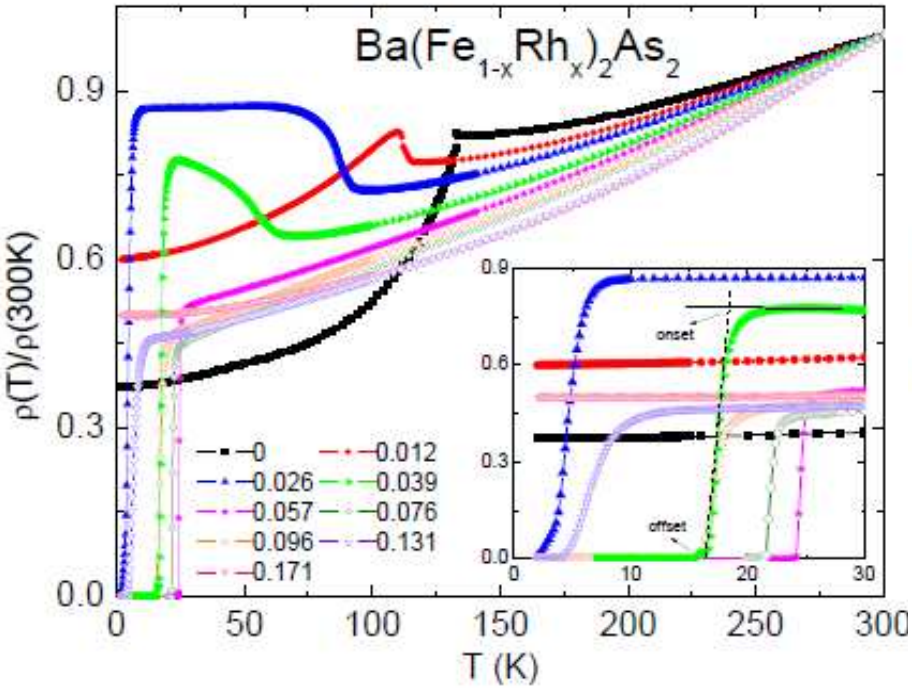


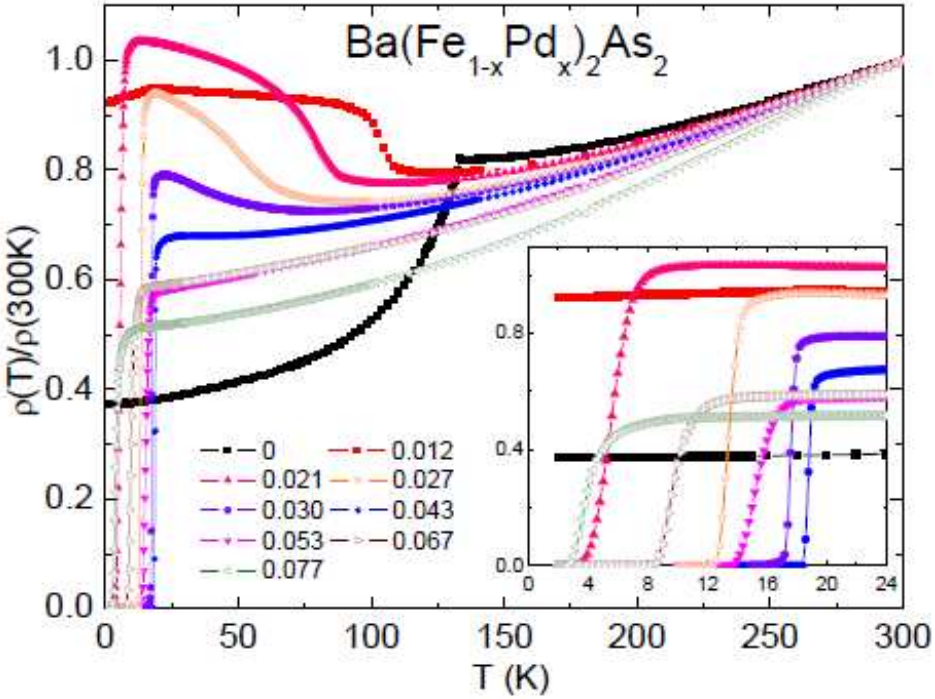
This can be further explored with the isoelectronic, 4d-TM doping series.

PHYSICAL REVIEW B **80**, 024511 (2009)

Phase diagrams of $Ba(Fe_{1-x}M_x)_2As_2$ single crystals (M=Rh and Pd)

N. Ni, A. Thaler, A. Kracher, J. Q. Yan, S. L. Bud'ko, and P. C. Canfield



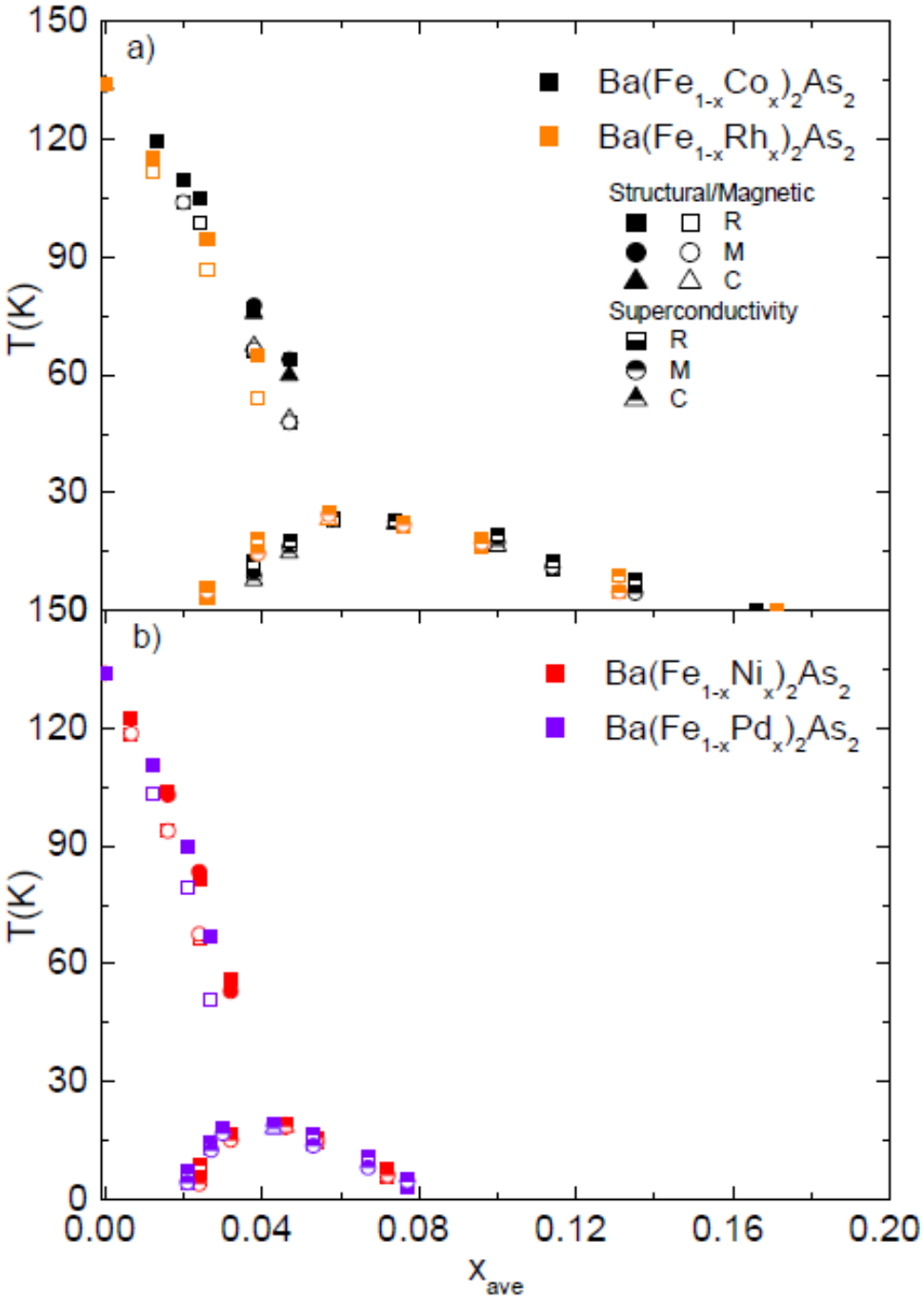


Using our thermodynamic and transport data (as well as the experimentally determined x values) we can construct T-x and T-e phase diagrams.

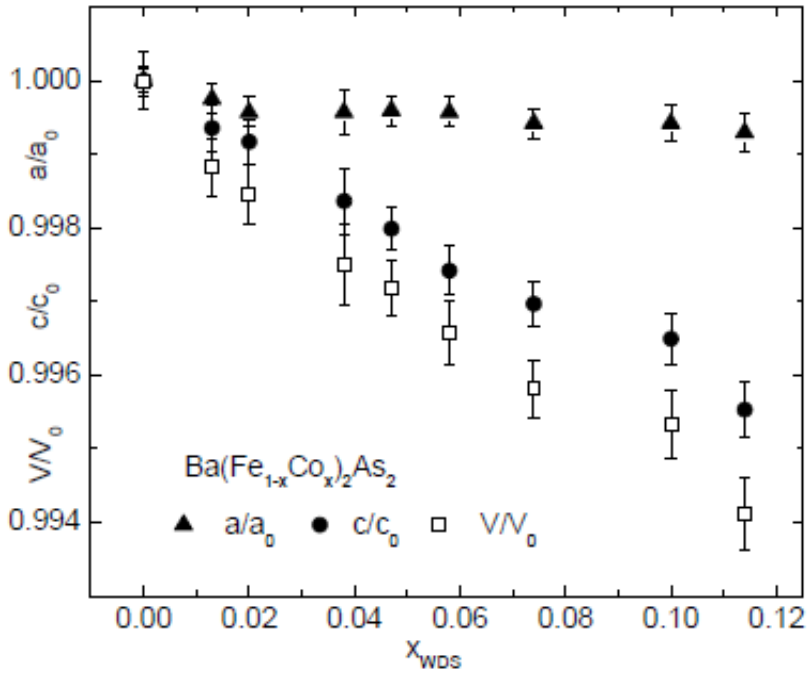
When we compare the isoelectronic Co- and Rh-doped series we find identical phase diagrams.

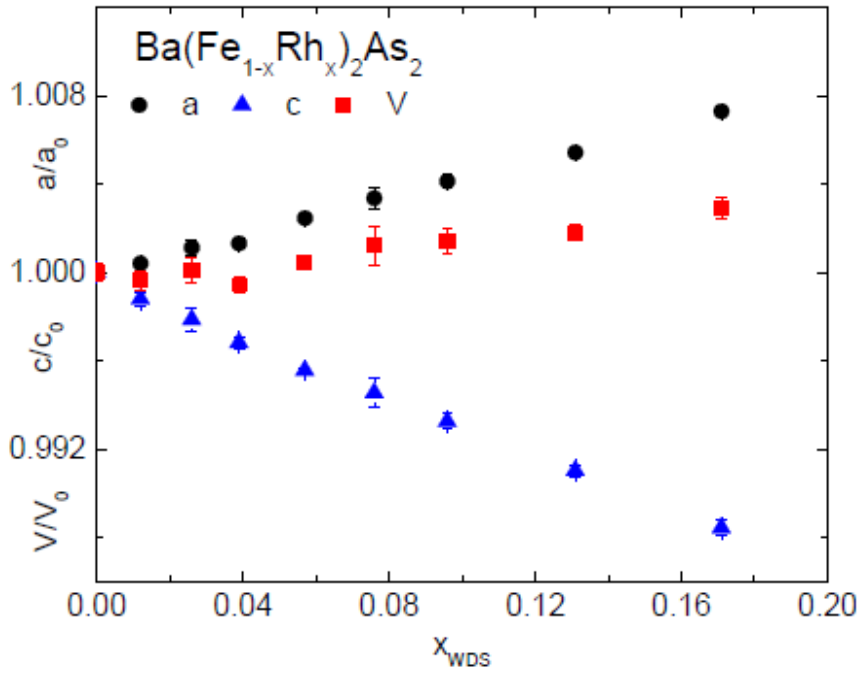
When we compare the isoelectronic Ni- and Pd-doped series we again find identical phase diagrams.

This remarkable similarity between the isoelectronic phase diagrams can only be appreciated if the actual x is determined. Nominal x-values differ from TM to TM' series.



PHYSICAL REVIEW B 80, 024511 (2009)





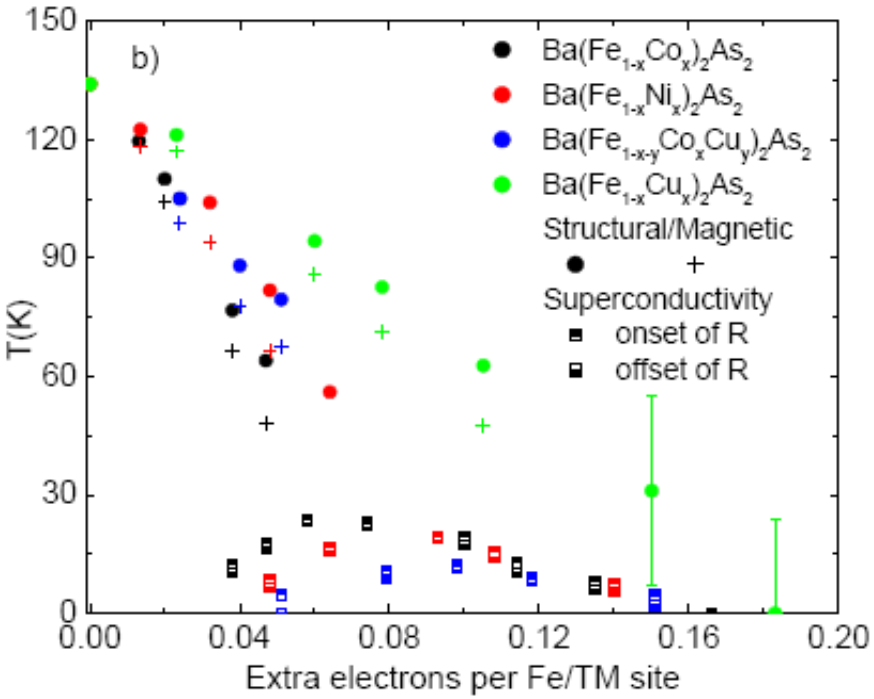
Although the phase Co- and Rh-doped phase diagrams are virtually identical, the effects of Co and Rh on the lattice parameters are very different.

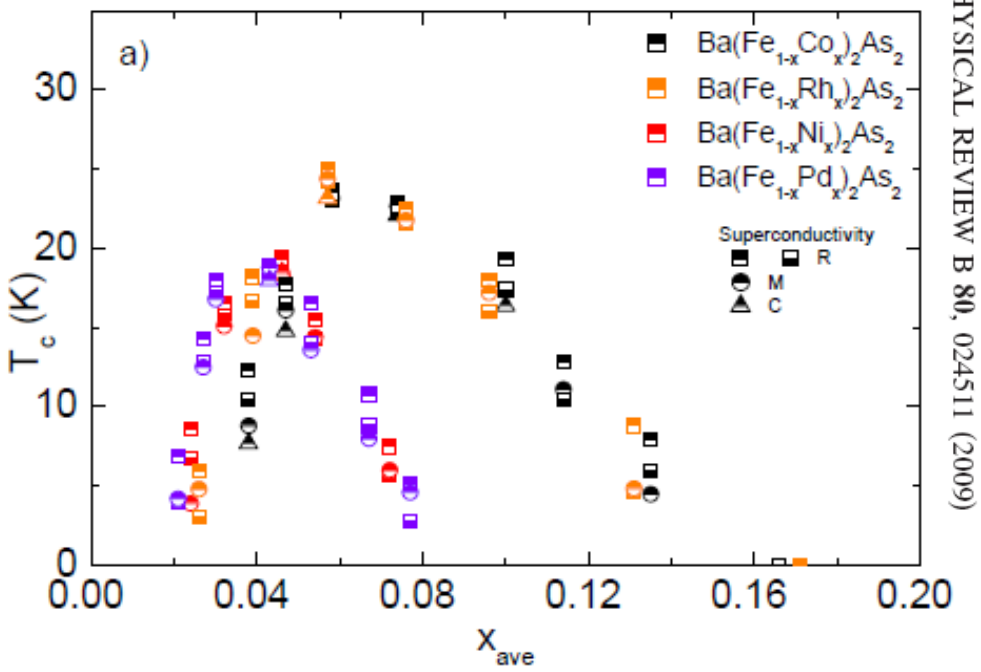
This implies that changes in lattice parameter are not the primary variable shifting the transition temperatures.

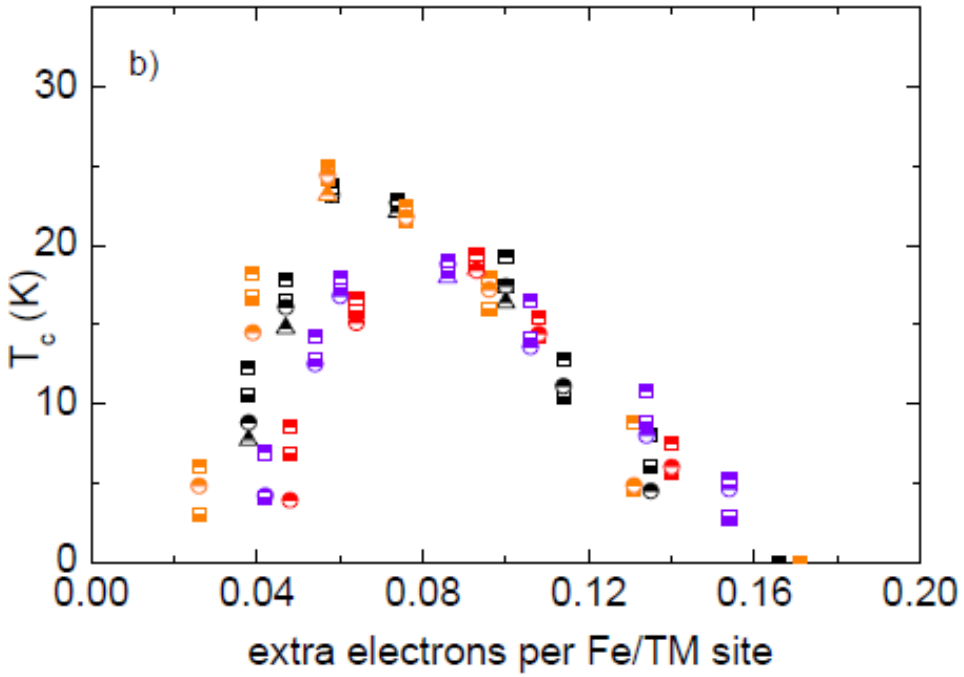
As will be show later, effects of pressure or isoelectronic substitution are much more gradual than what we see when we add extra electrons.

PHYSICAL REVIEW B **82**, 024519 (2010)

We can now examine the T_c dome is greater detail. There is excellent scaling of T_c with e on the over doped side. On the under-doped side, there is a variation that is associated with how far we have suppressed the upper transitions.



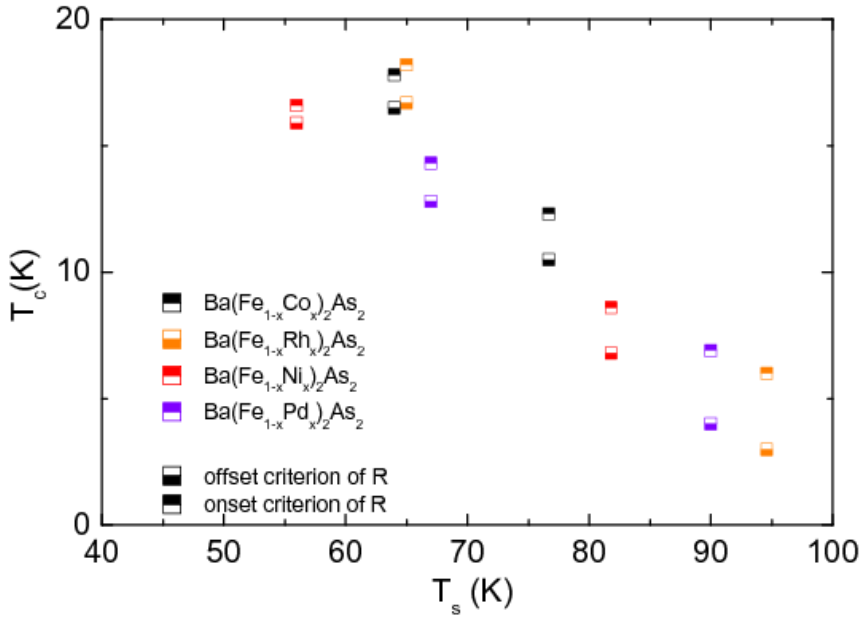


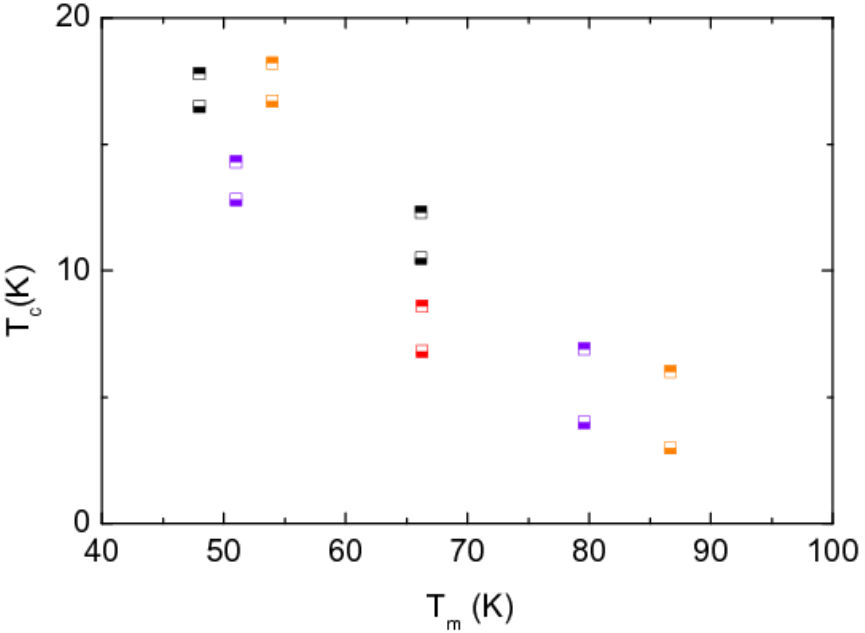


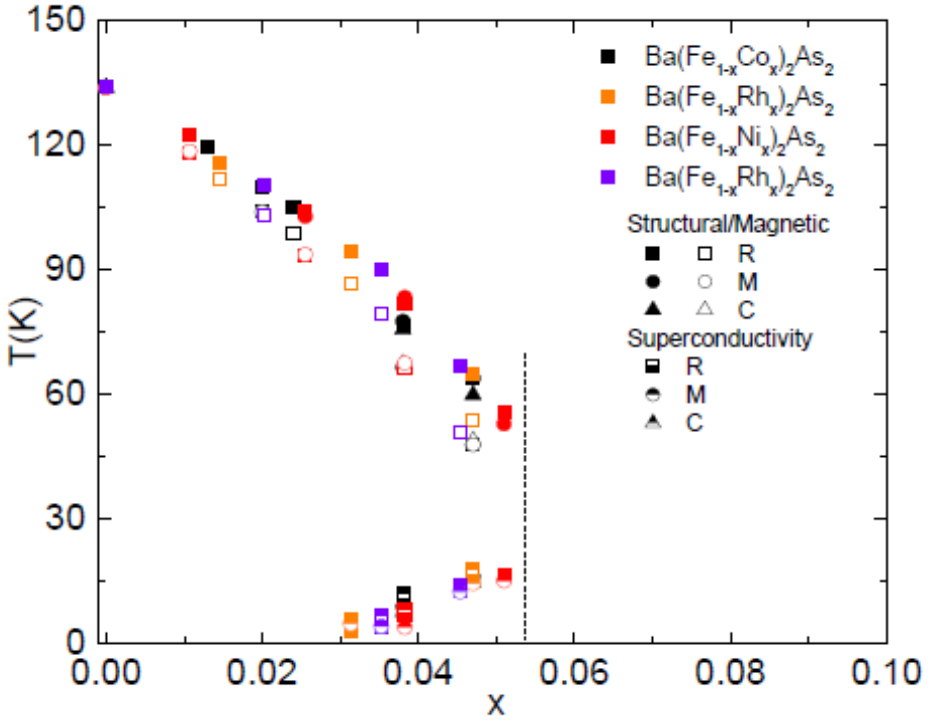
PHYSICAL REVIEW B 80, 024511 (2009)

Plots of $T_c(T_s)$ and $T_c(T_m)$ clearly reveal the correlation between T_c and the suppression of these higher temperature transition. This is again indicating that there is a competition between these states

If we normalize the suppression of the upper transitions we see that all of the T_c curves collapse onto a single manifold.





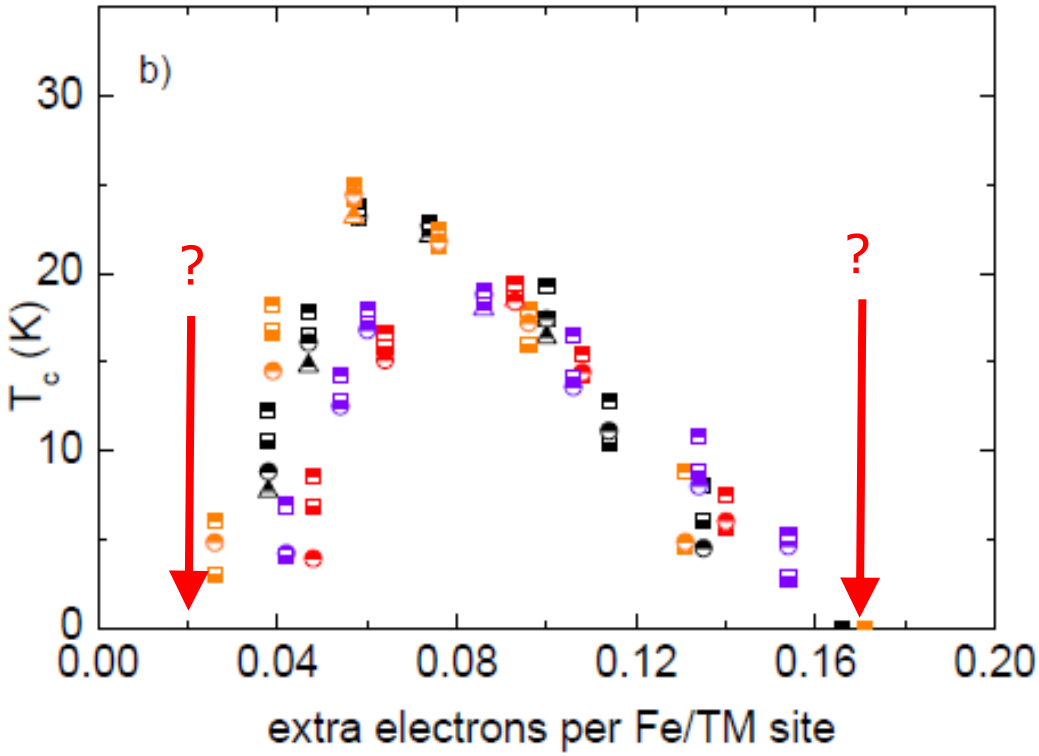


PHYSICAL REVIEW B 80, 024511 (2009)

Basic Questions:

How do we understand scaling with "e" and what determines the extent of the superconducting dome?

The answers were found in TEP, Hall and ARPES measurements.



PHYSICAL REVIEW B **80**, 054517 (2009)

Thermoelectric power and Hall coefficient measurements on $Ba(Fe_{1-x}T_x)_2As_2$ (T=Co and Cu)

Eun Deok Mun, Sergey L. Bud'ko, Ni Ni, Alex N. Thaler, and Paul C. Canfield
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(Received 6 June 2009; revised manuscript received 5 August 2009; published 26 August 2009)

Evidence for a Lifshitz transition in electron-doped iron arsenic superconductors at the onset of superconductivity

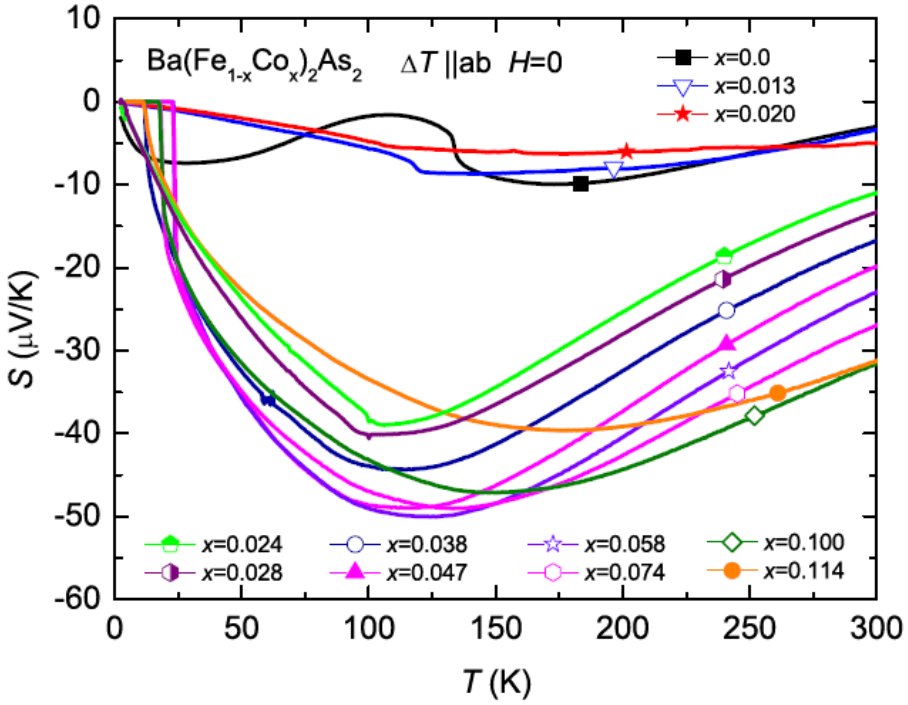
nature physics

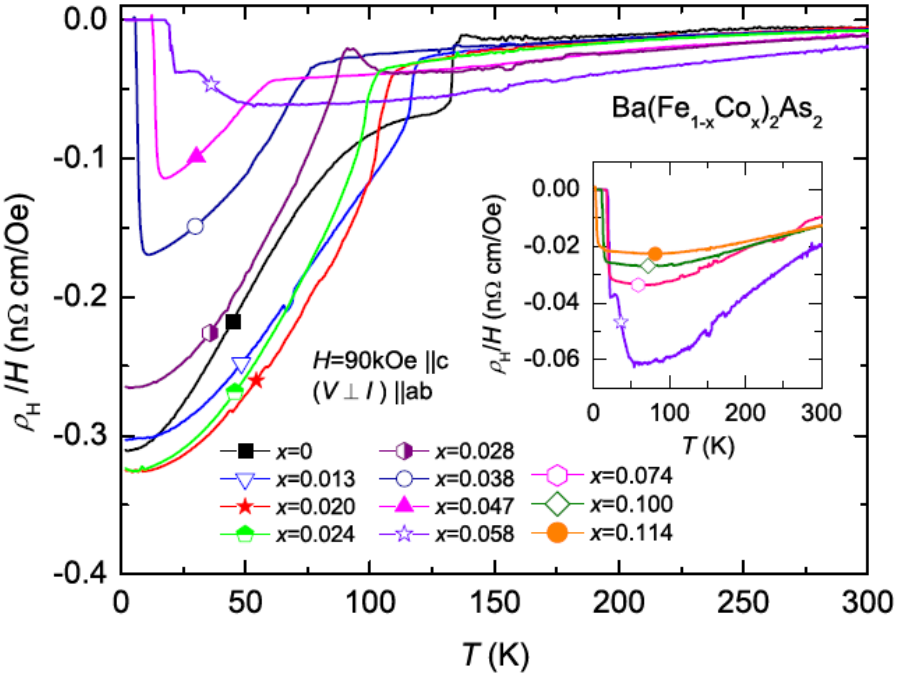
NATURE PHYSICS | VOL 6 | JUNE 2010 | www.nature.com/naturephysics 419

We measured the TEP and Hall coefficient for Co doped $BaFe_2As_2$, with specifically high density on the low Co-doped side.

There is a dramatic change in TEP over the whole temperature range measured as x crossed from 0.02 to 0.024

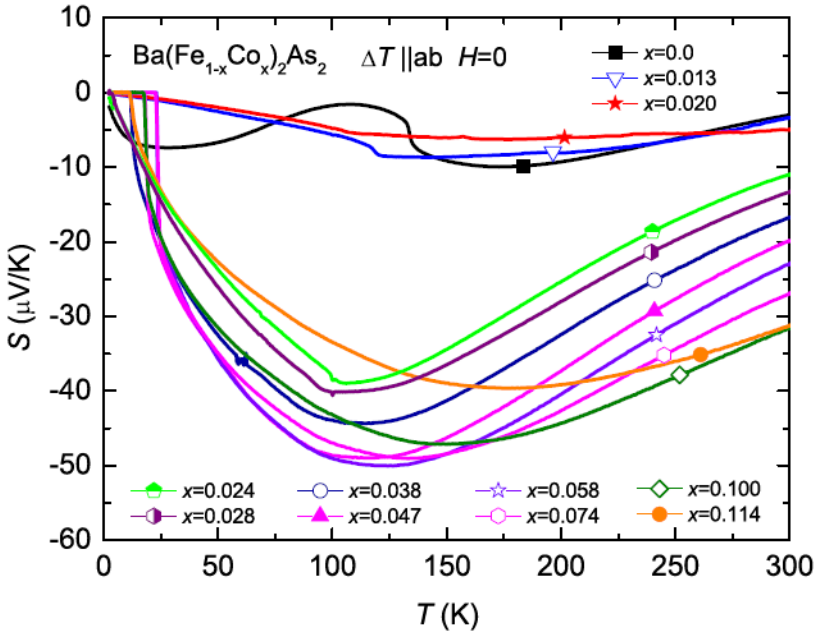
The low temperature Hall coefficient changes for the same x values.

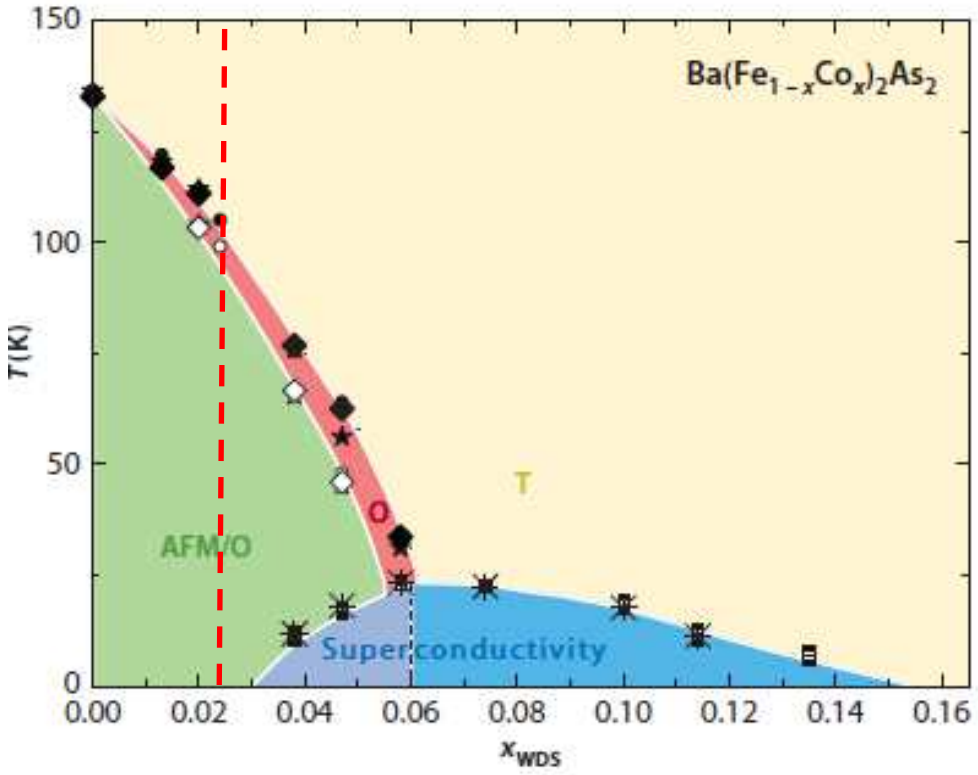




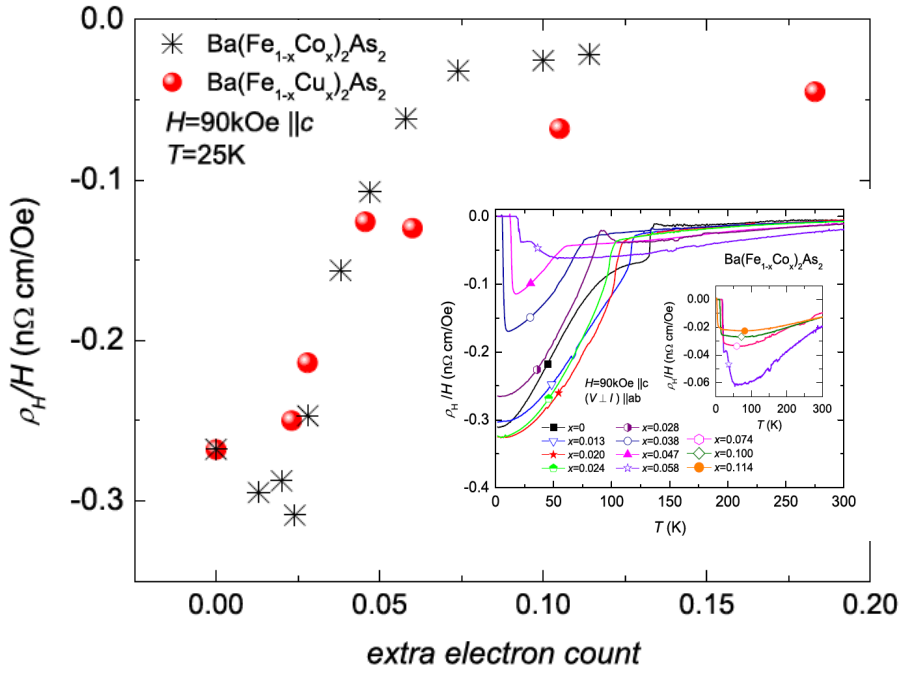
PHYSICAL REVIEW B 80, 054517 (2009)

Both the TEP and ρ_H/H data show a sharp change for x (e) ~ 0.025 . For Co doped $BaFe_2As_2$ this is just before the onset of the supercond. dome.

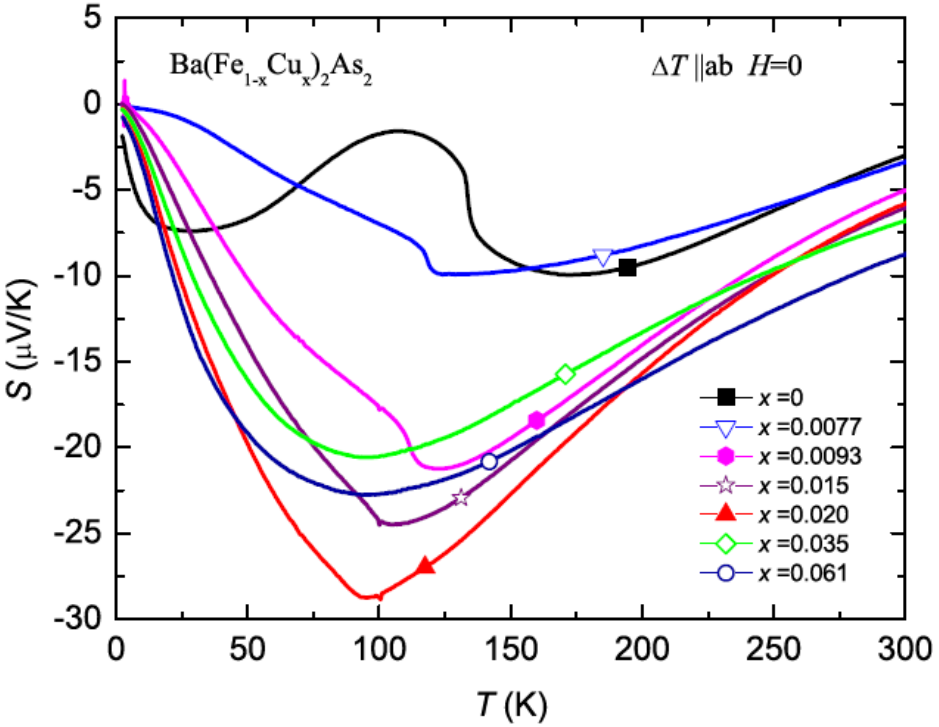


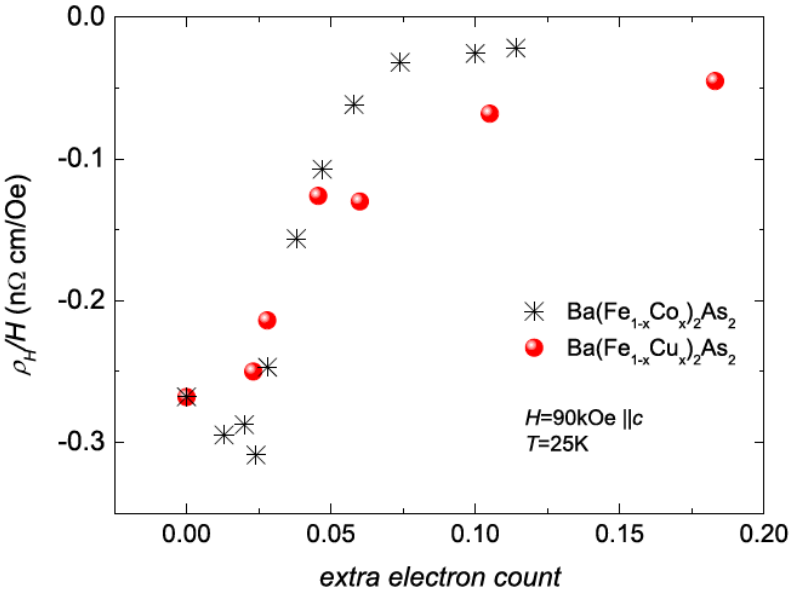


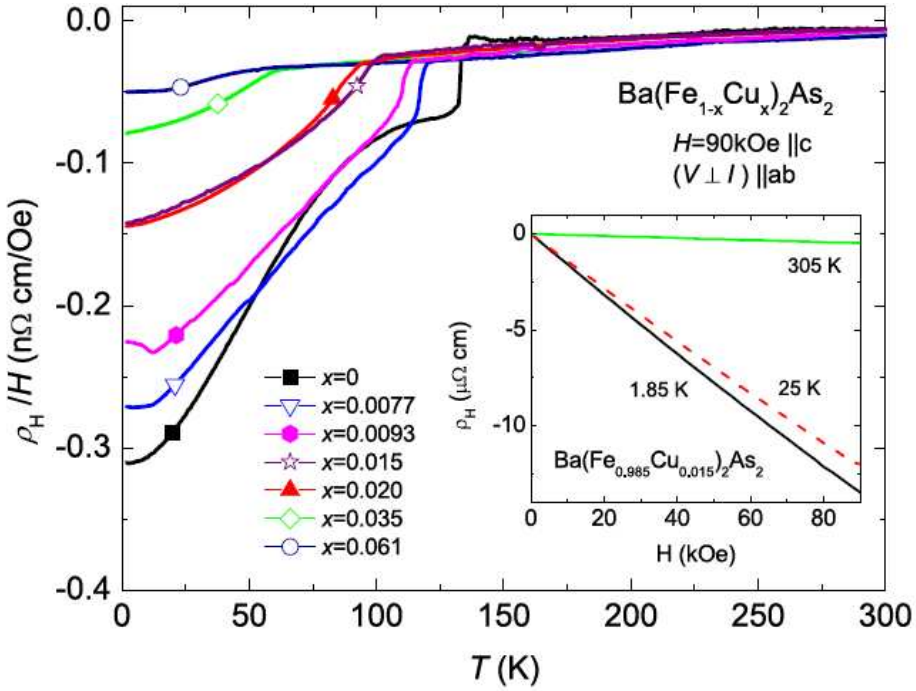
PHYSICAL REVIEW B 80, 054517 (2009)



The same changes can be seen in the TEP and Hall data for Cu doping, at the same e-count, e ~ 0.025. The fact that such a similar change occurs at the same e-value further supports the idea that Cu changes the system three times more rapidly than Co does.



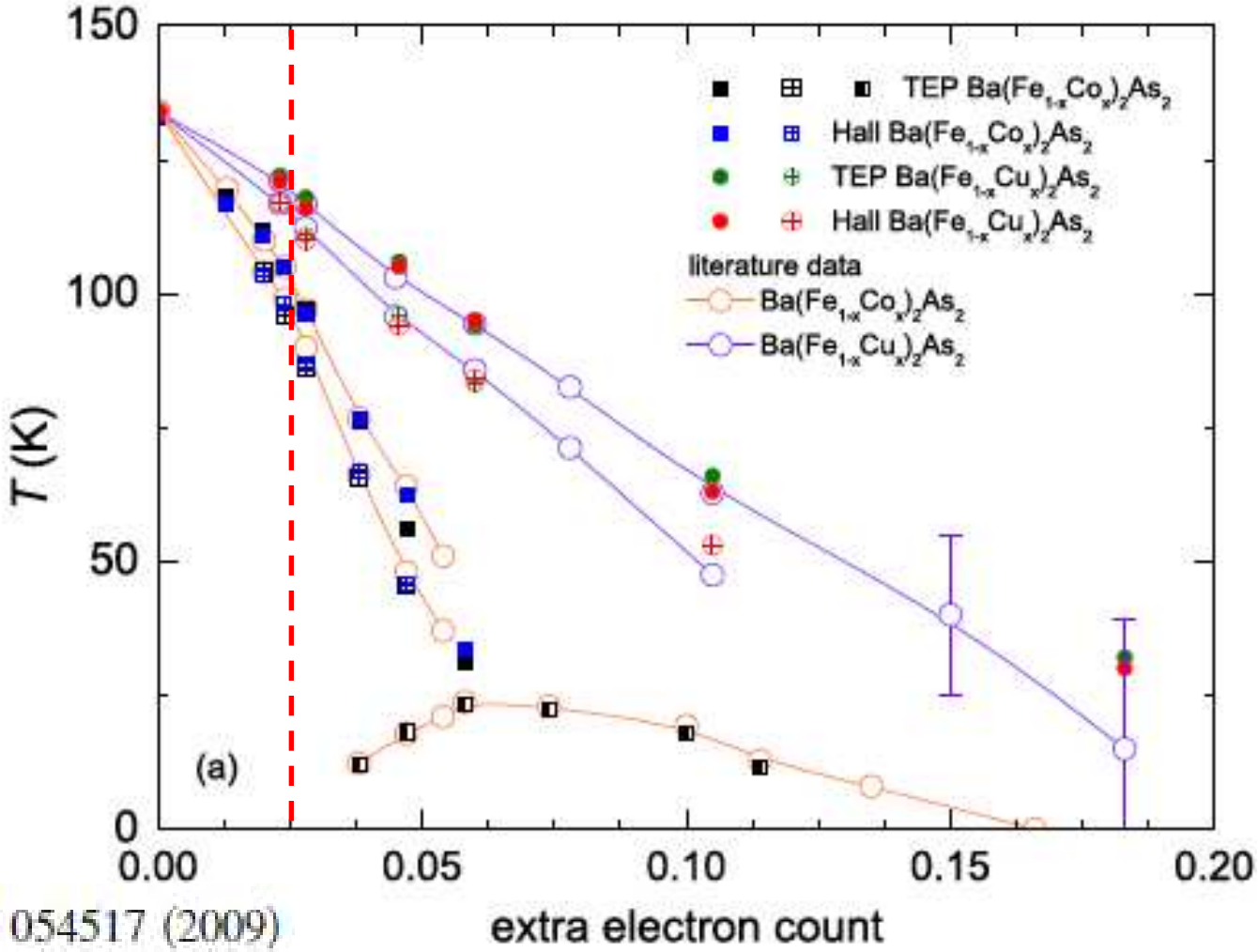




PHYSICAL REVIEW B 80, 054517 (2009)

These data are consistent with the idea that there is a change in the band structure or Fermi surface of $BaFe_2As_2$ for small e-doping (e.g. a Lifshitz transition) and it happens independently of the existence of superconductivity.

If so, then this should be apparent in ARPES measurement….



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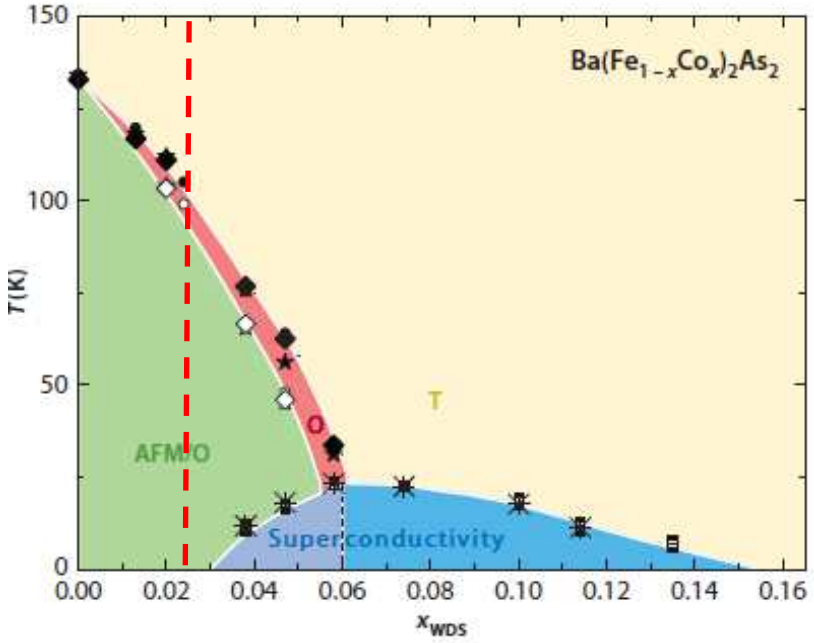
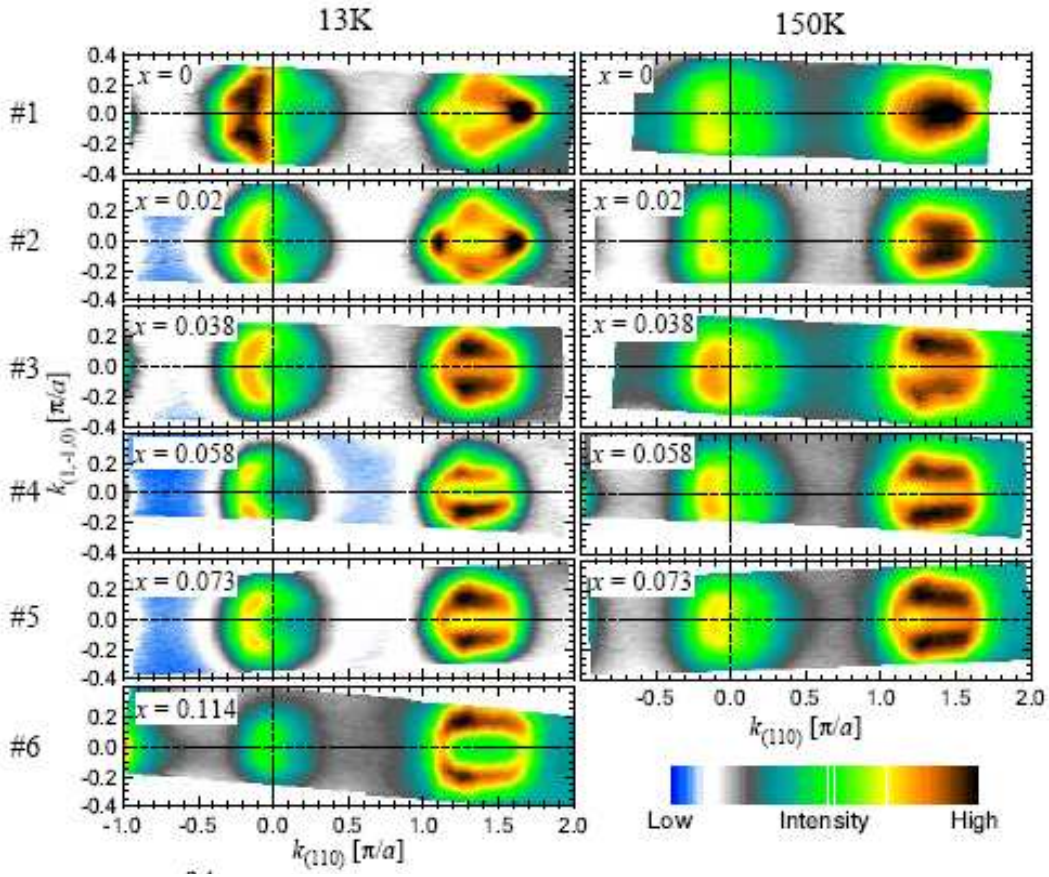
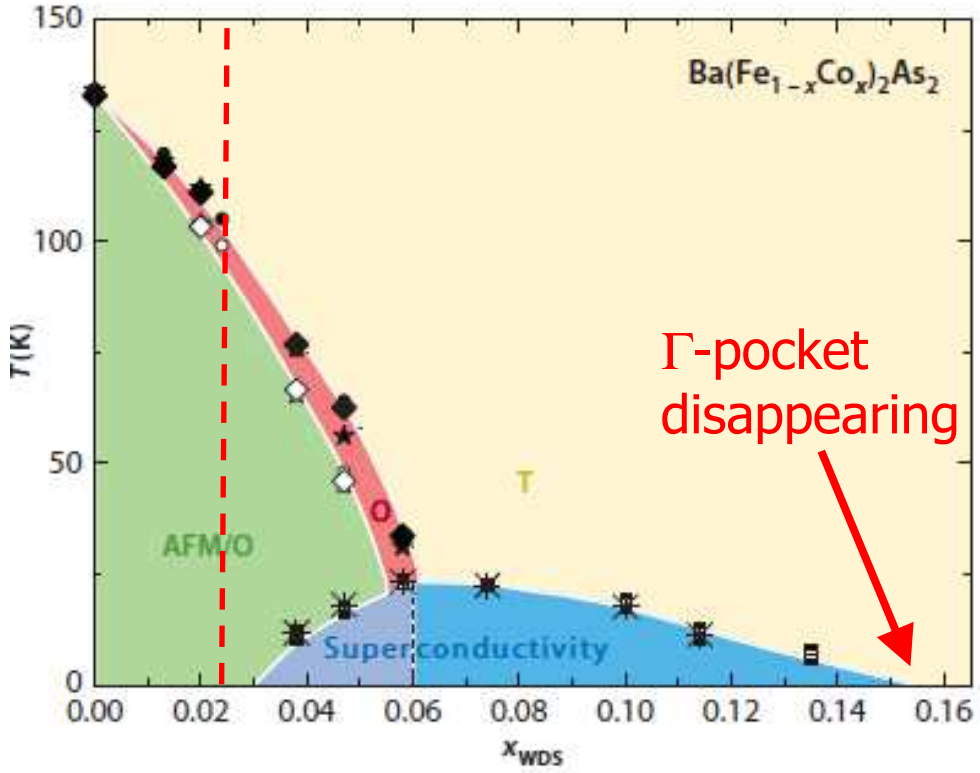
ARPES data taken across the Co-doped $BaFe_2As_2$ series show a suppression of the reconstruction of the FS in the AF state as well as a qualitative change in the 150 K FS for x >~ 0.025

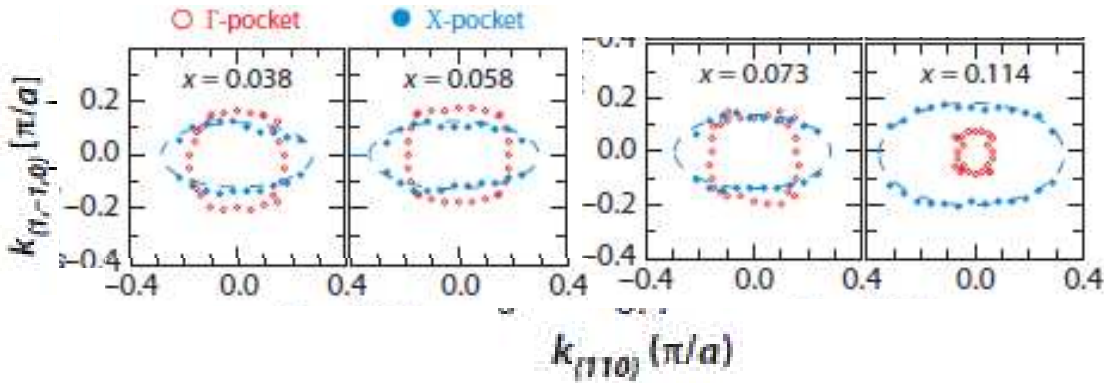


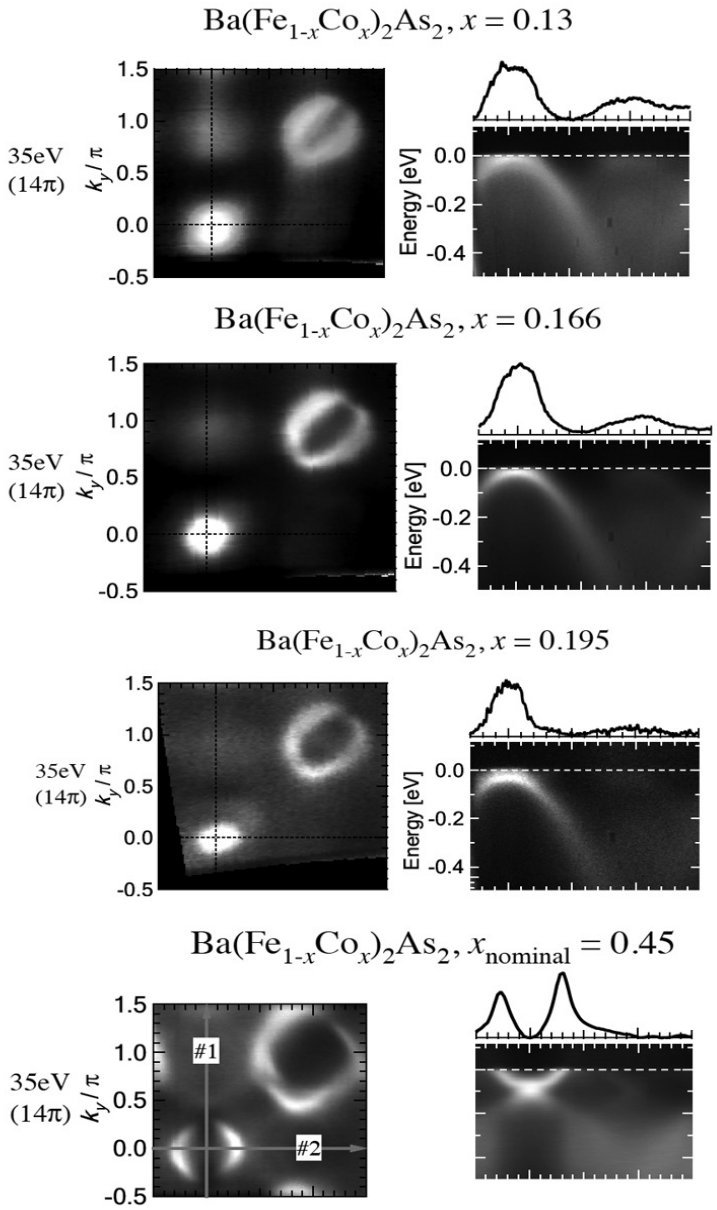


Chang Liu…Adam Kaminski, et al.

In addition it becomes clear that T_c does not vitally depend upon nesting but does depend on the size of the shrinking hole pocket.







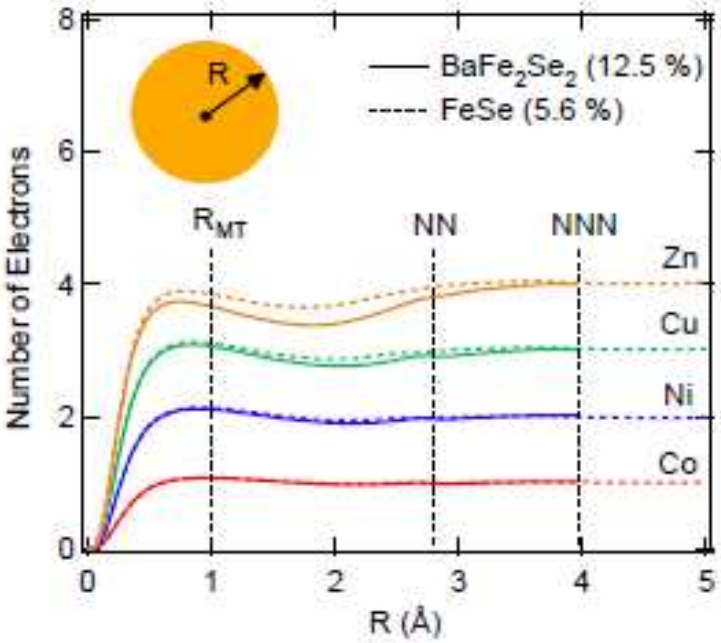
Finally, e may not be band filling….

Where Are the Extra *d* Electrons in Transition-Metal Substituted Fe Pnictides?

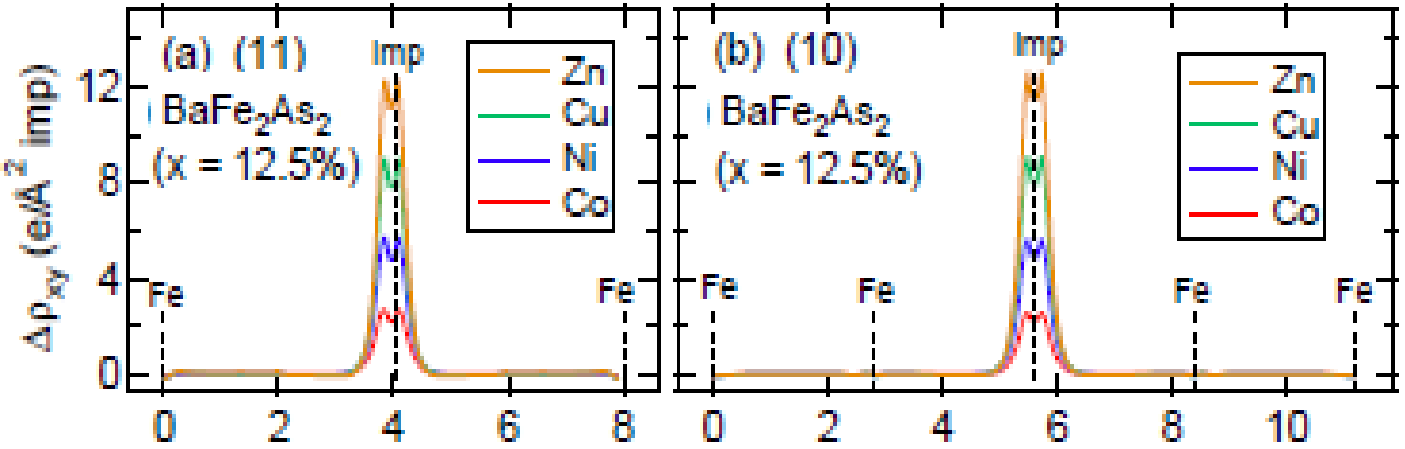
H. Wadati,[1] I. Elfimov,[2] and G. A. Sawatzky[1,*]

arXiv:1003.2663v1 [cond-mat.supr-con] 13 Mar 2010

In a very recent posting it is suggested (based on density functional theory calculations) that the extra electrons stay highly localized around the impurity atoms and act as scatters and "wash out part of the Fermi surface by 'scrambling k-space' ". While this an interesting and potentially appealing idea it needs to incorporate 4d doping data and ARPES results.



NOTE: This model preserves Ni=2xCo and Cu=3xCo trend we see in data too.



Clearly simple e-value (or band filling) is not everything…there are other ways of tuning the band structure…. *There is pressure*

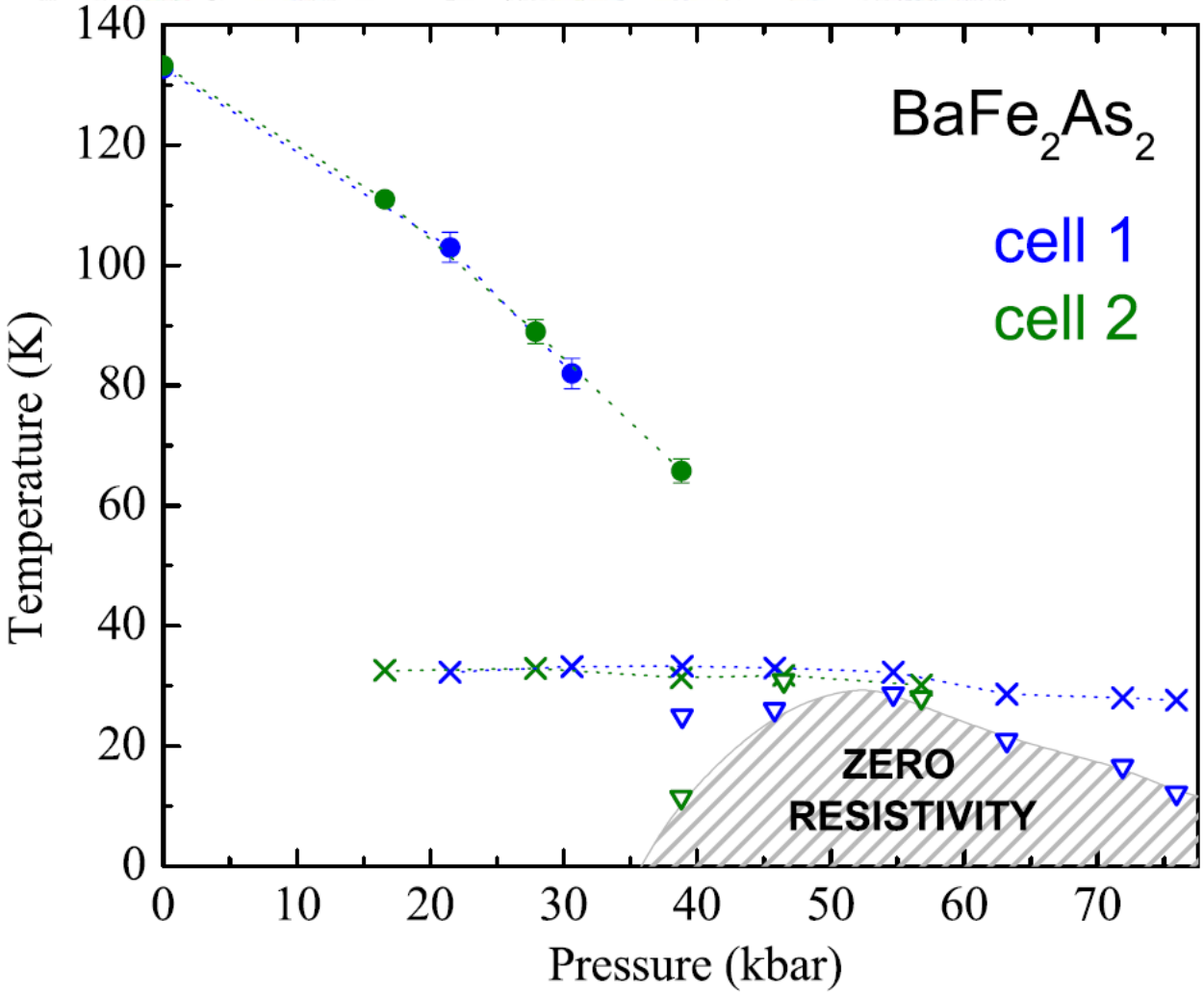
PHYSICAL REVIEW B 79, 224518 (2009)

Complete pressure-dependent phase diagrams for $SrFe_2As_2$ and $BaFe_2As_2$

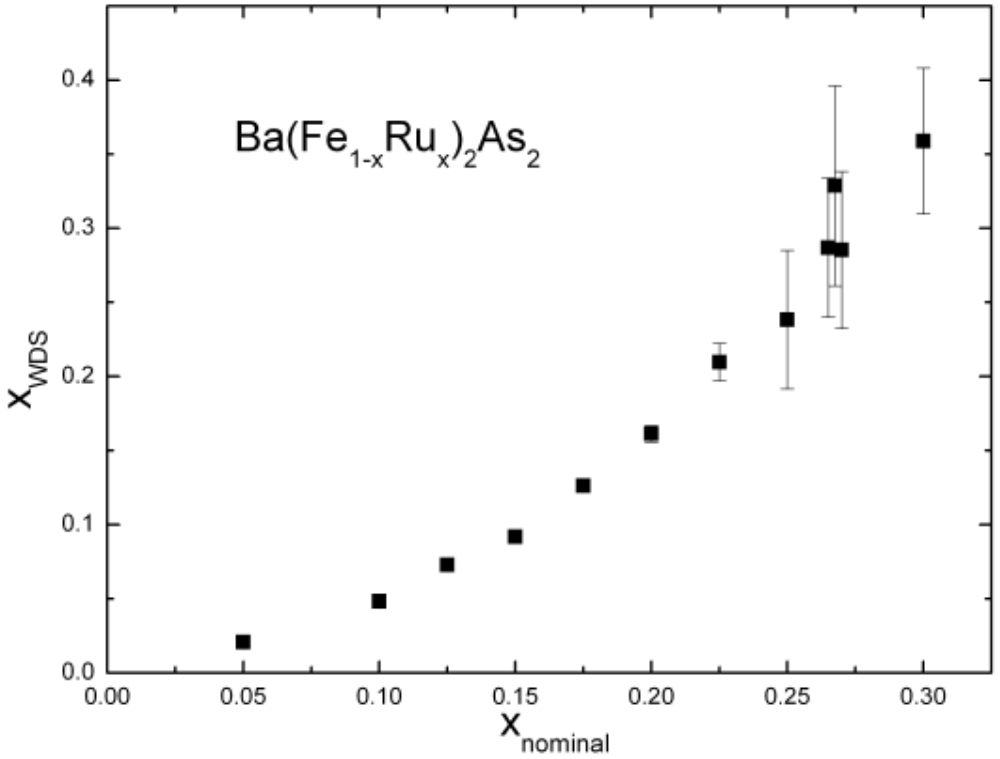
E. Colombier, S. L. Bud'ko, N. Ni, and P. C. Canfield

Although we have taken advantage of TM doping to tune $BaFe_2As_2$, there are other ways of revealing similar phase diagrams. Applied pressure suppresses the structural / magnetic phase transition and reveals a superconducting dome as well.

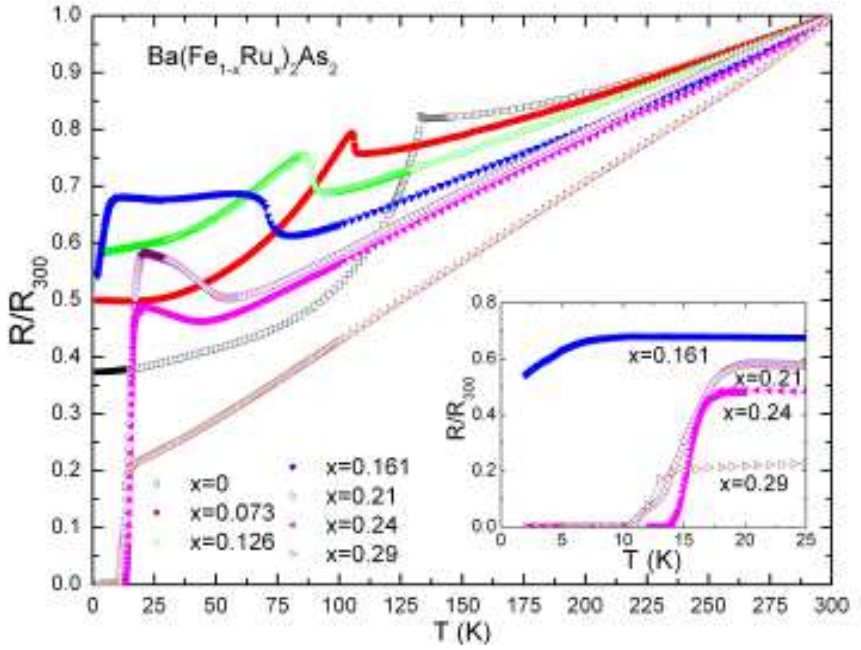
One hypothesis is that doping and pressure change band structural feature in a similar manner



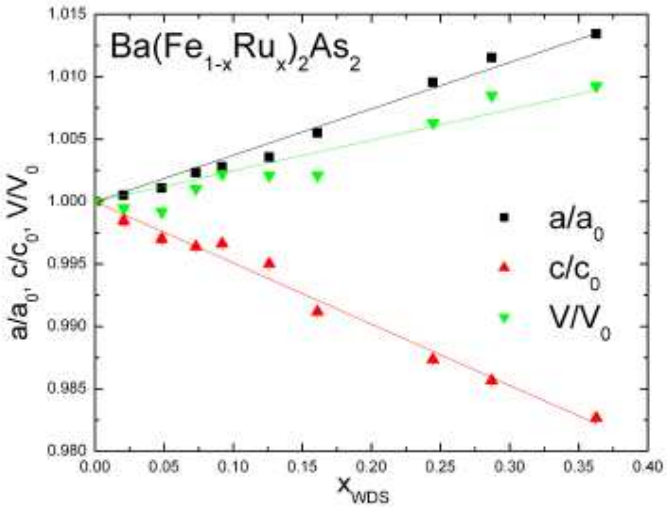
Clearly simple e-value (or band filling) is not everything…there are other ways of tuning the band structure…. *There is also Ru (isoelectronic)*



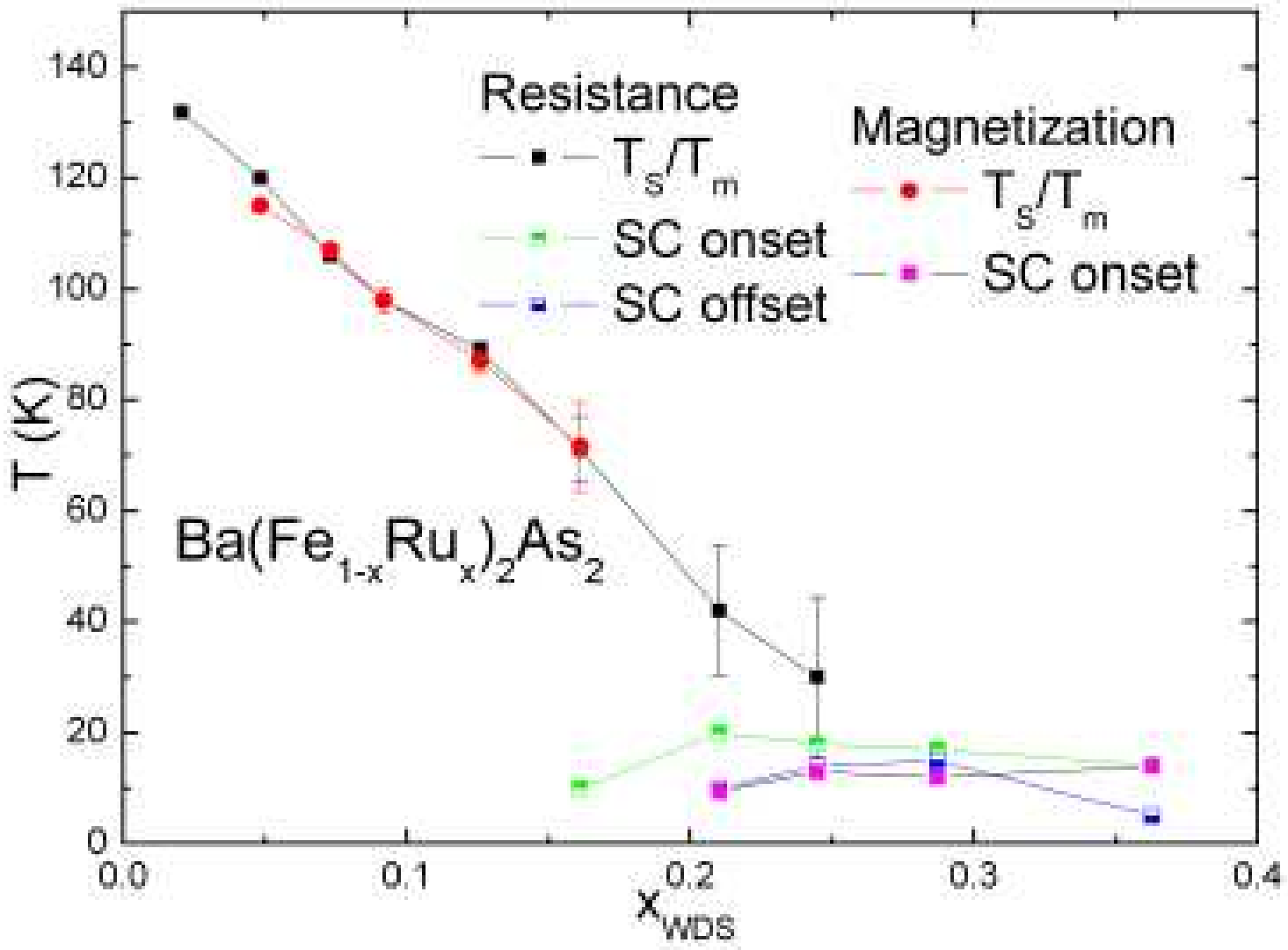
PHYSICAL REVIEW B 82, 014534 (2010)



$Ba(Fe_{1-x}Ru_x)_2As_2$											
N	14	16	12	12	11	19	18	13	14	15	25
$x_{nominal}$	0.05	0.1	0.125	0.15	0.175	0.2	0.225	0.25	0.265	0.27	0.3
x_{WDS}	0.021	0.048	0.073	0.092	0.126	0.161	0.210	0.24	0.29	0.29	0.36
2σ	0.001	0.001	0.001	0.003	0.003	0.005	0.013	0.05	0.05	0.05	0.05

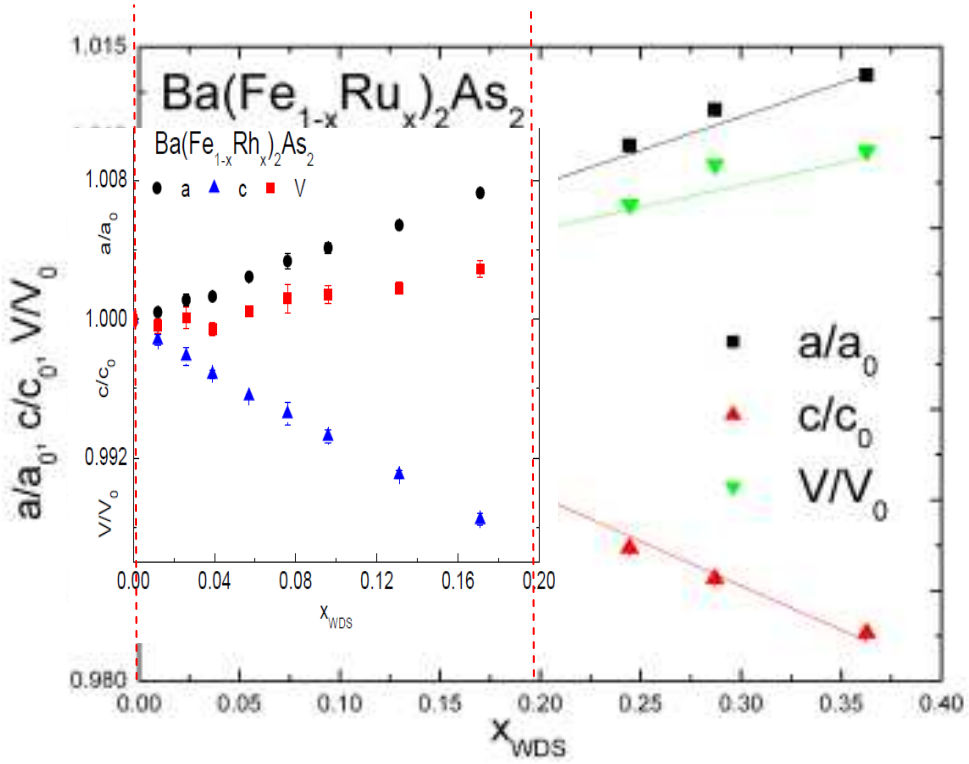


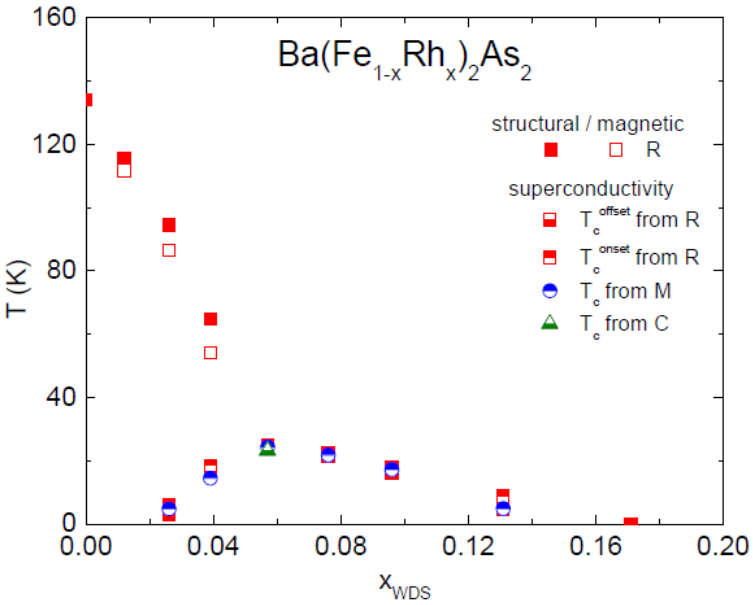
As before, we can assemble a phase diagram for Ru-doping. It is similar in that the signature of the structural / magnetic phase transition is suppressed and superconductivity appears close to the point where $T_{S/M}$ extrapolates to zero.

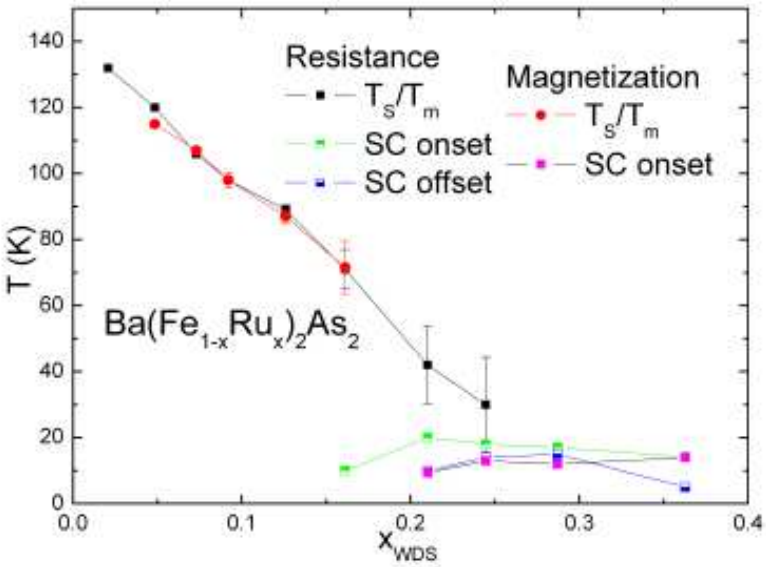


PHYSICAL REVIEW B 82, 014534 (2010)

The changes in the unit cell dimensions and volume are remarkably similar for Ru and Rh. On the other hand, the phase diagrams are very different. This demonstrates that there is a very clear difference between "steric" and electronic effects.



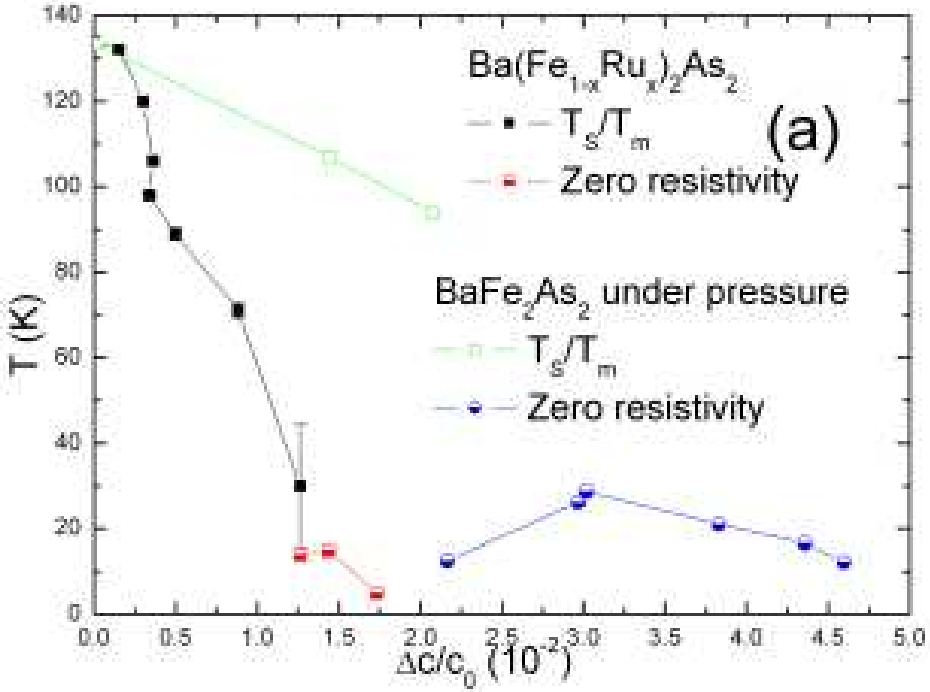




It takes a lot more change in lattice parameter for isoelectronic substitution to suppress $T_{S/M}$ and lead to T_c

PHYSICAL REVIEW B 82, 014534 (2010)

Ru doping bears a much stronger resemblance to tuning with pressure. This is show qualitatively below and quantitatively to the right where changes in the c-axis parameter may "catch" the salient physics.



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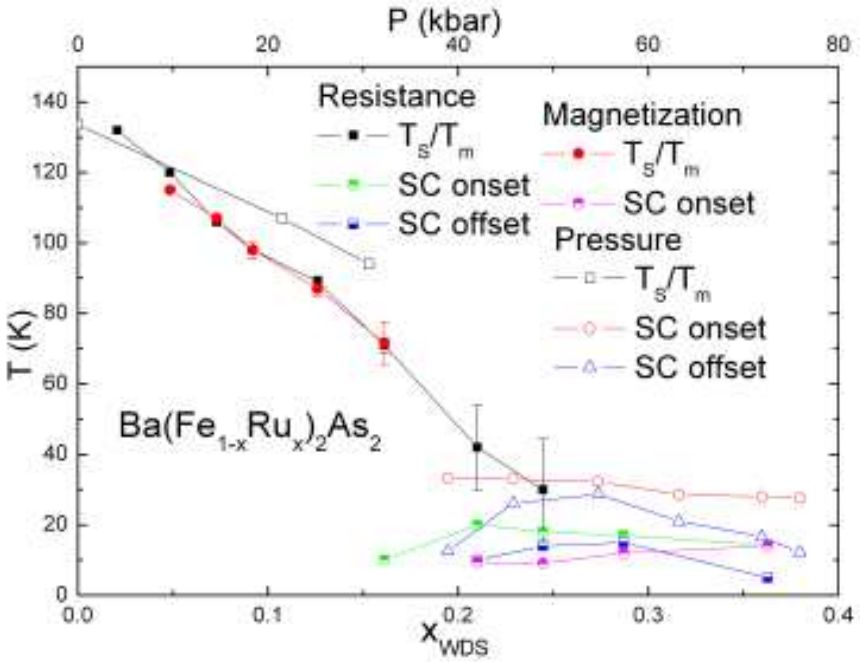
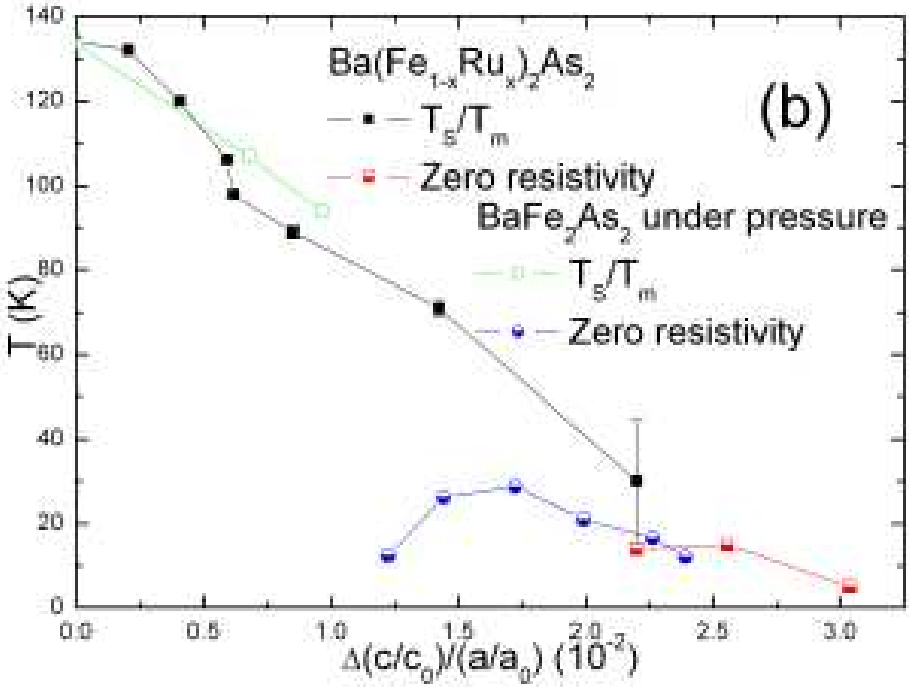
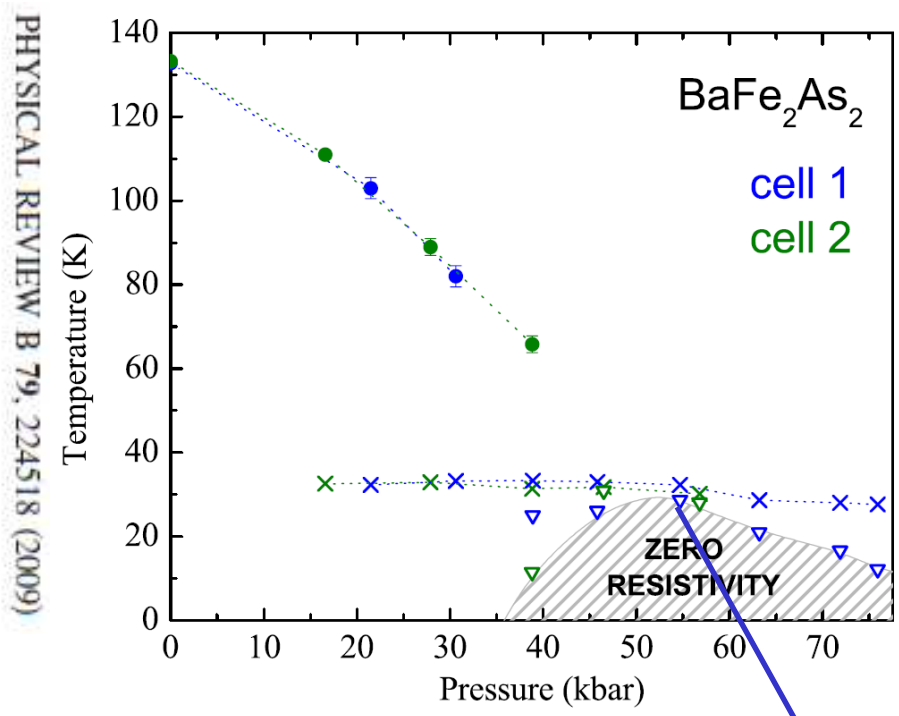
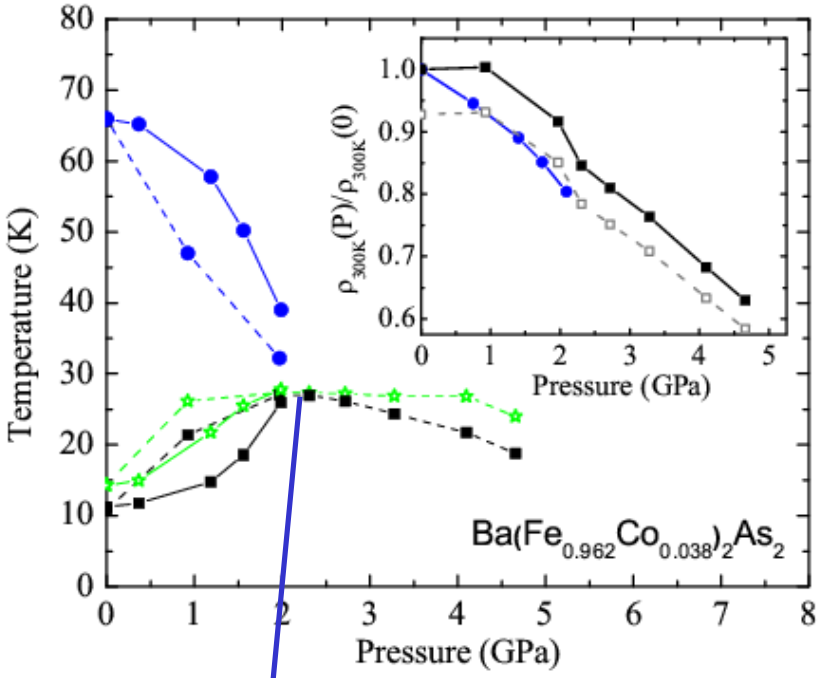
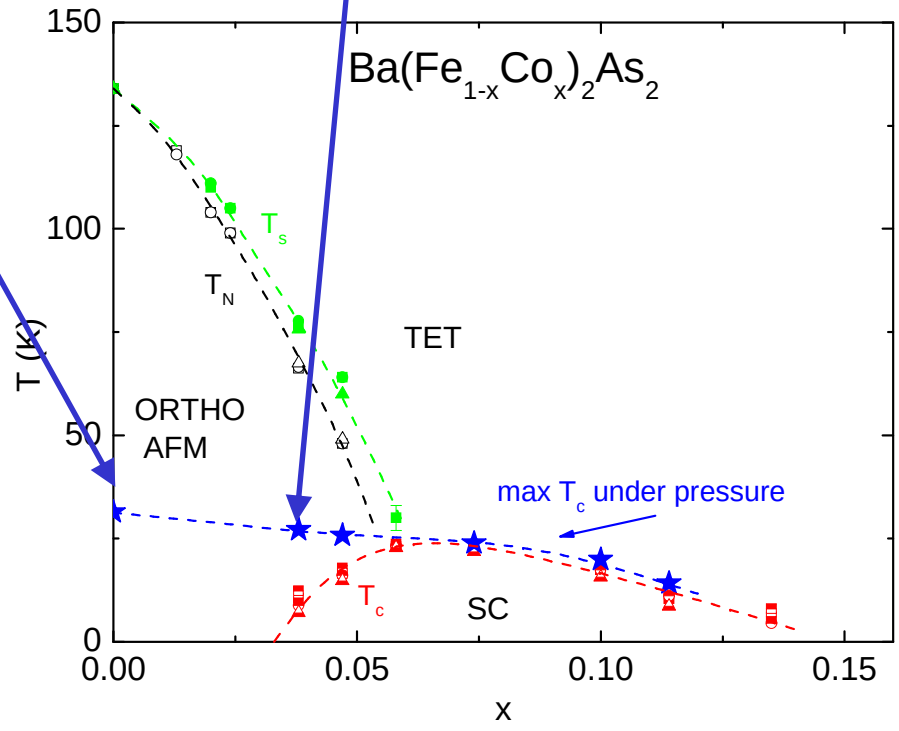






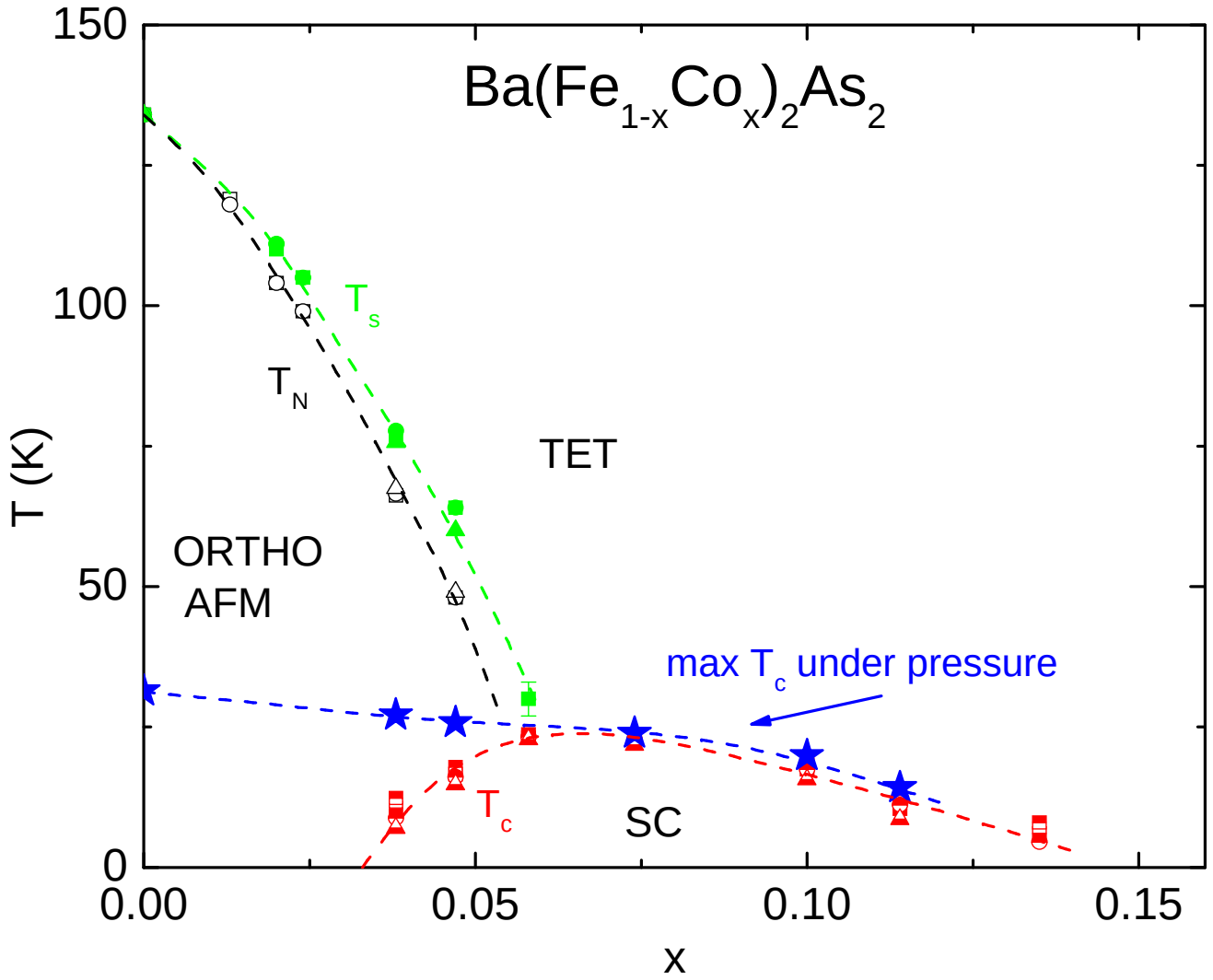




We have recently measured the effect of pressure on samples across the Co-doped $BaFe_2As_2$ series. We find that on the under doped side pressure can increase T_c dramatically but does little to increase T_c on the overdoped side of the dome.

Pressure seems to be primarily suppressing the structural / magnetic phase transitions and "allowing" superconductivity to reach its full potential (or reach maximum T_c). Once T_M/T_S is suppressed by doping pressure only gradually suppresses T_c and does not increase T_c-max.

This plot again emphasizes the competition between T_s/T_m and T_c. It also shows that the Co-doped $BaFe_2As_2$ system could support even higher T_c values if T_s/T_m could be suppressed more rapidly.



By studying $Ba(Fe_{1-x}TM_x)_2As_2$ series for a variety of 3d- and 4d-TM dopants we have found that:

(i) The structural / antiferromagnetic phase transition is suppressed in a similar manner for all TM and scales roughly with x.

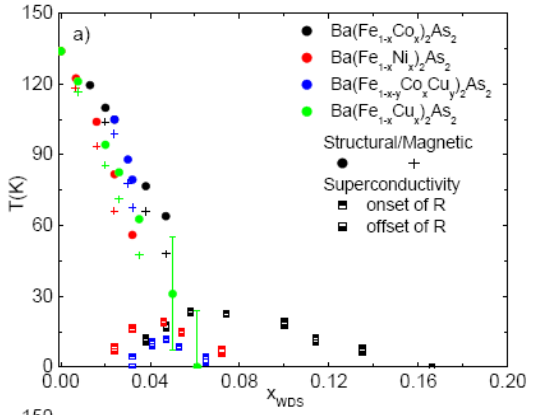
(ii) There is a region of e that supports super-conductivity if the structural / antiferromagnetic phase transition is suppressed sufficiently.

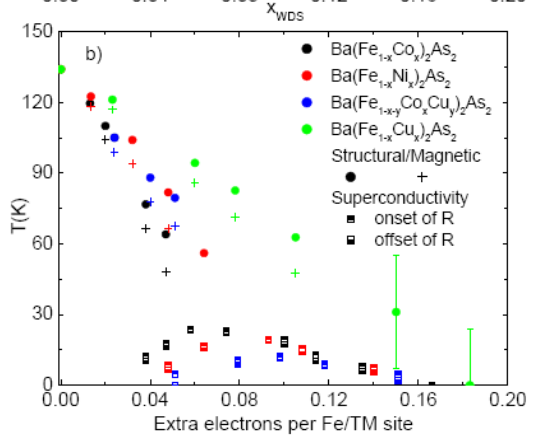
(iii) The superconducting dome scales very well with e on the over-doped, tetragonal phase, side.

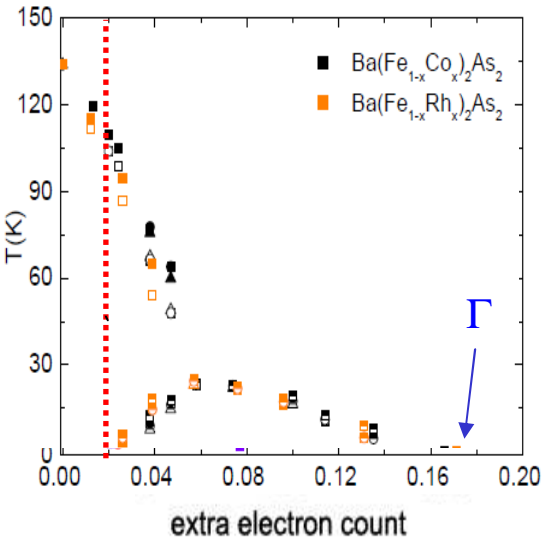
(iv) The onset of the superconducting dome on the under-doped, O / AF side depends on how quickly the upper transitions are suppressed. T_c scales well with T_S and / or T_M.

(v) The limits of the extent of the superconducting dome are set by band structural features on both the low and high e-value sides.

(vi) The effects of pressure are subtly different, suppressing $T_{S/M}$ without adding electrons.





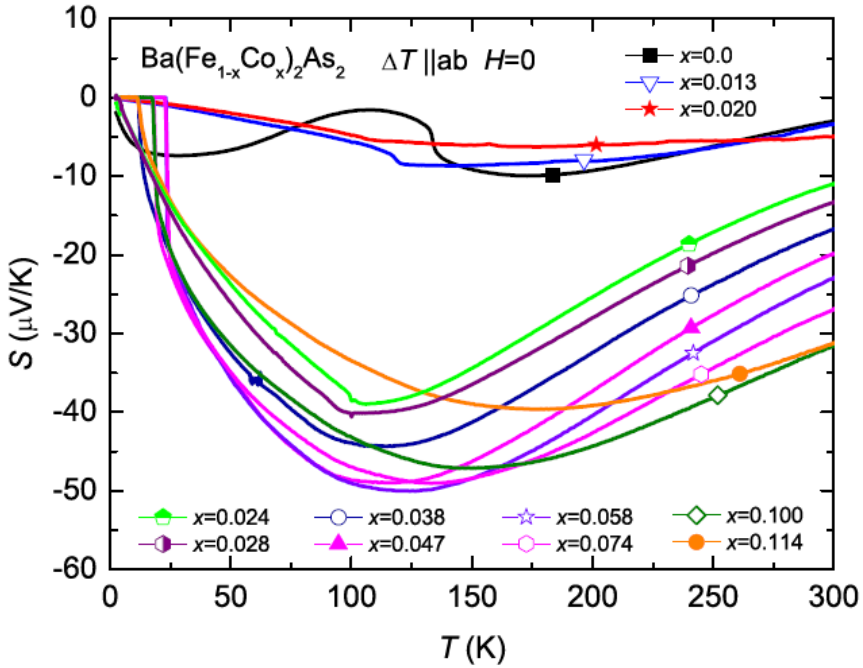


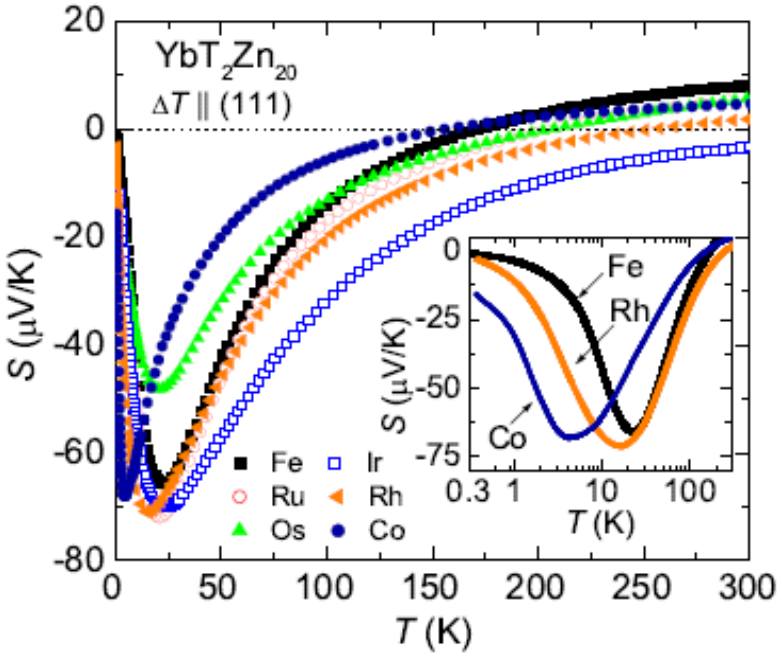
A couple of open questions (possibly even key points):

There is repeated evidence (phase diagram as well as TEP/Hall) that Cu effects change three times as fast (Ni two times as fast) as Co. What is the origin of these changes: band filling, scattering, something else?

Plot ratio of S / Cp and see entropy per carrier

The dramatic change in TEP as Co is doped into $BaFe_2As_2$ is remarkable. Suddenly the FeAs material has TEP comparable to Yb-based heavy fermion. What is this telling us? What is difference between pure and doped materials?






That's All Folks

“A towel, it says, is about the most massively useful thing an interstellar hitchhiker can have. Partly it has great practical value. You can wrap it around you for warmth as you bound across the cold moons of Jaglan Beta; you can lie on it on the brilliant marble-sanded beaches of Santraginus V, inhaling the heady sea vapors; you can sleep under it beneath the stars which shine so redly on the desert world of Kakrafoon; use it to sail a miniraft down the slow heavy River Moth; wet it for use in hand-to-hand-combat; wrap it round your head to ward off noxious fumes or avoid the gaze of the Ravenous Bugblatter Beast of Traal (such a mind-bogglingly stupid animal, it assumes that if you can't see it, it can't see you); you can wave your towel in emergencies as a distress signal, and of course dry yourself off with it if it still seems to be clean enough.

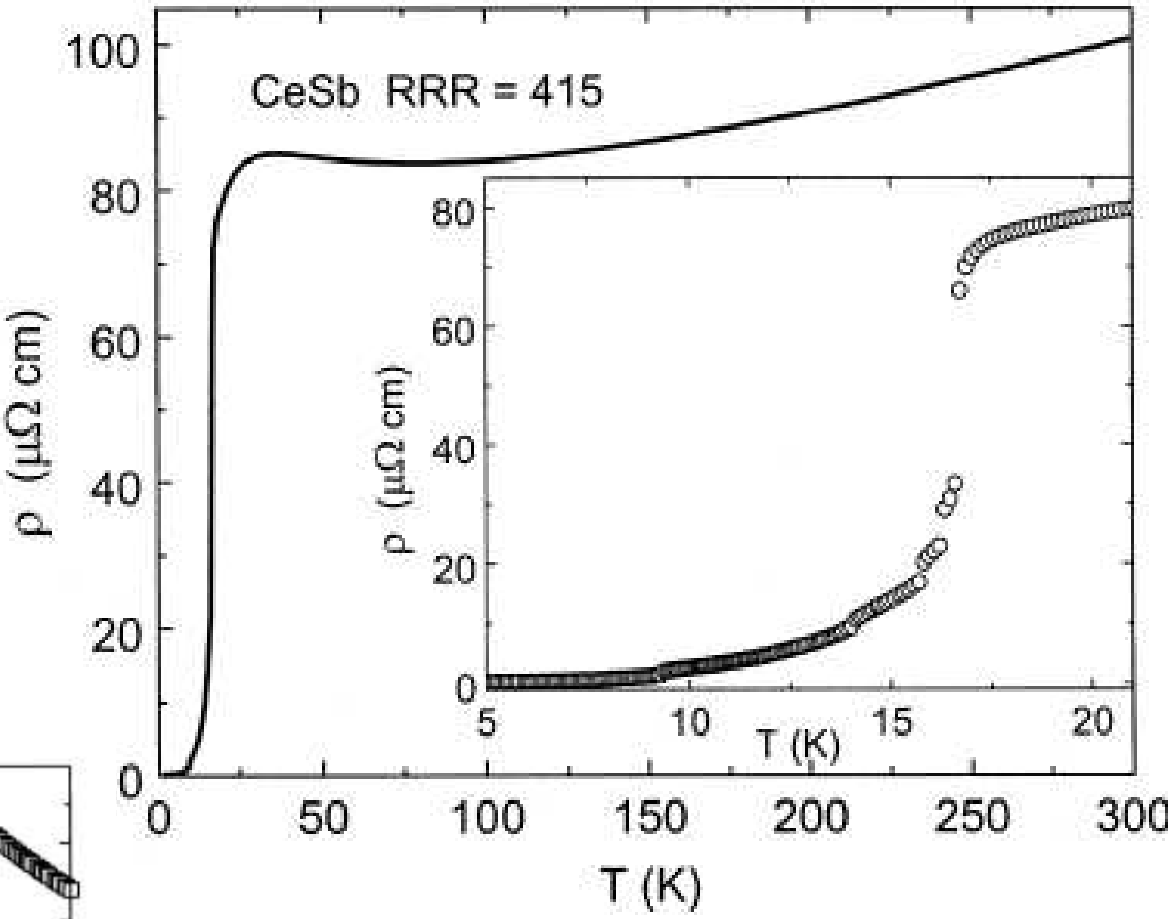
More importantly, a towel has immense psychological value. For some reason, if a strag (strag: non-hitch hiker) discovers that a hitch hiker has his towel with him, he will automatically assume that he is also in possession of a toothbrush, face flannel, soap, tin of biscuits, flask, compass, map, ball of string, gnat spray, wet weather gear, space suit etc., etc. Furthermore, the strag will then happily lend the hitch hiker any of these or a dozen other items that the hitch hiker might accidentally have "lost". What the strag will think is that any man who can hitch the length and breadth of the galaxy, rough it, slum it, struggle against terrible odds, win through, and still knows where his towel is is clearly a man to be reckoned with.”

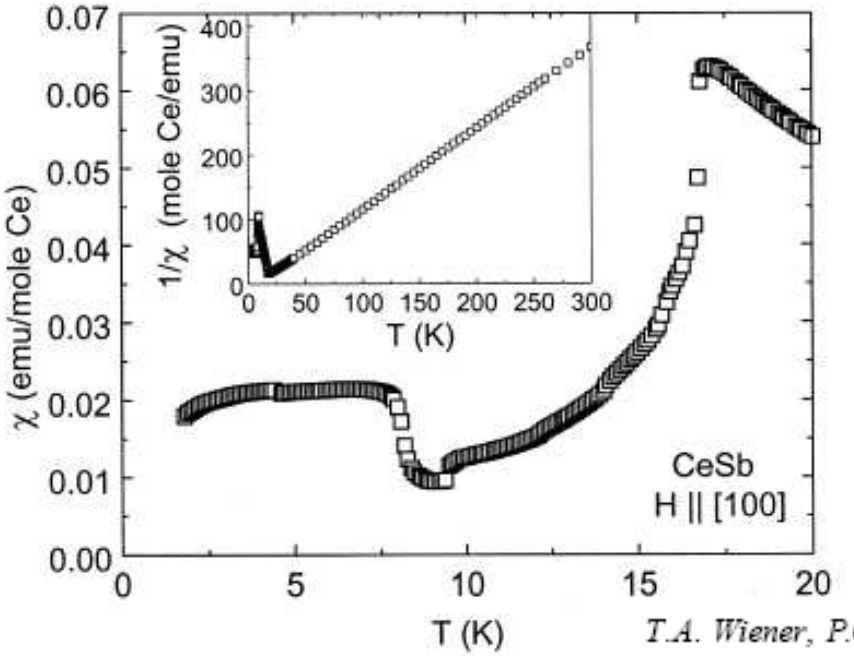
— Douglas Adams, *The Hitchhiker's Guide to the Galaxy*

Multiple transitions in temperature and field

CeSb

CeSb can be grown in exquisite purity from Sn flux. At first glance ρ and χ data seem to be a bit noisy at low T….





Actually CeSb has a formidable number of phase transition in zero and applied field and excellent (Sn flux grown) crystals allow us to examine them in detail.

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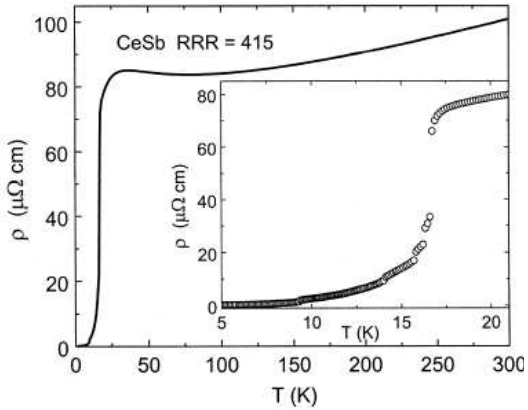
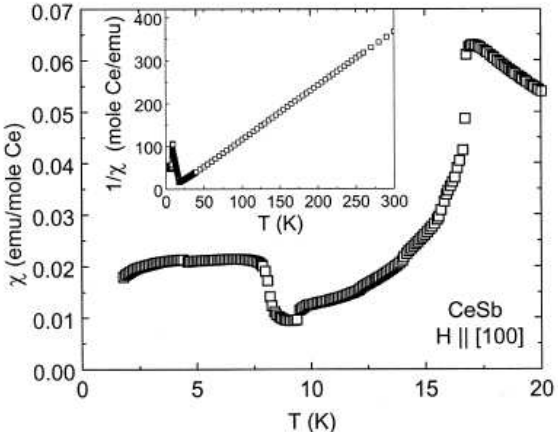
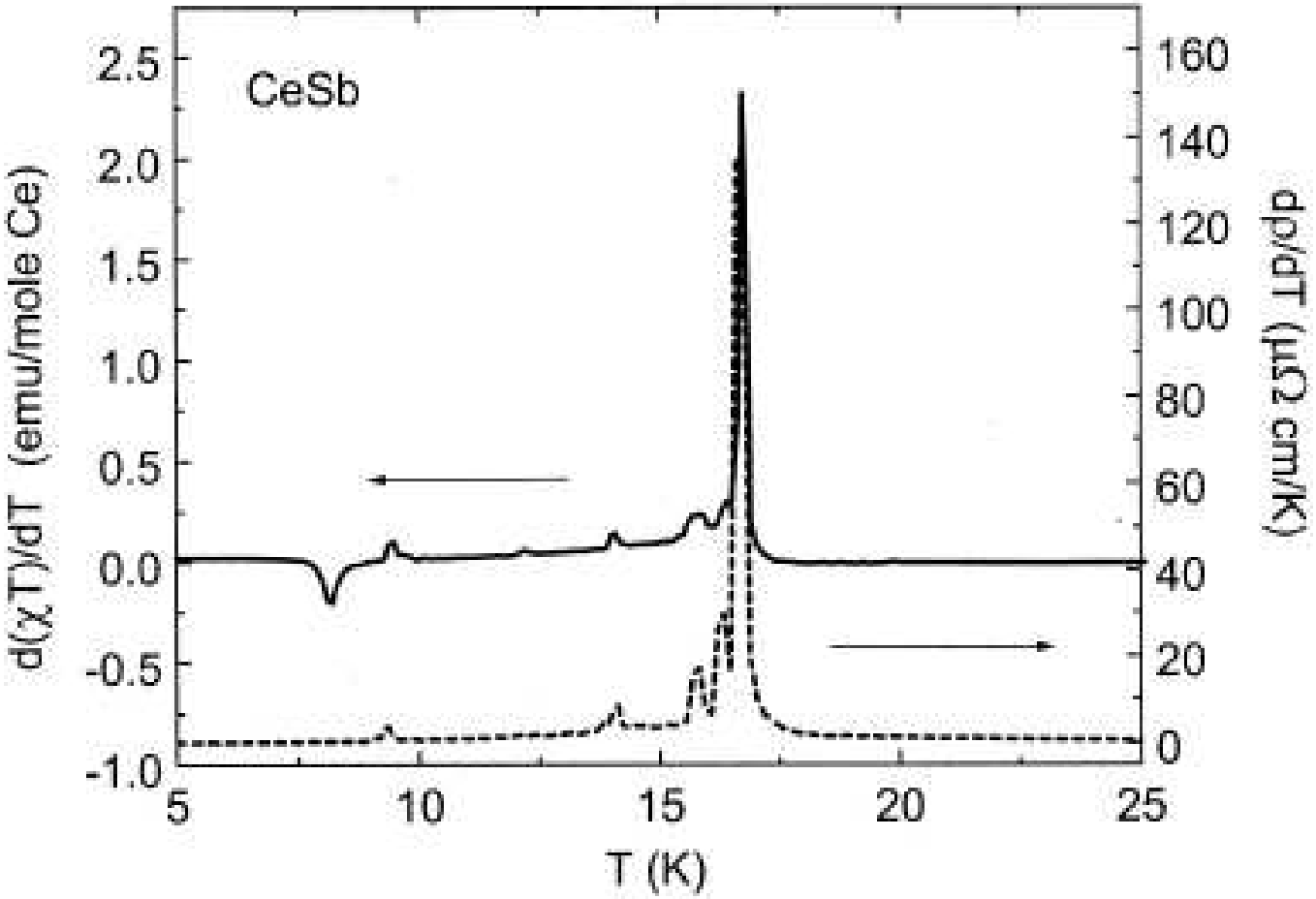
CeSb



Both χ and ρ data reveal a multitude of transitions.





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Multiple transitions in temperature and field

CeSb

These multiple transition appear in finite field as well.

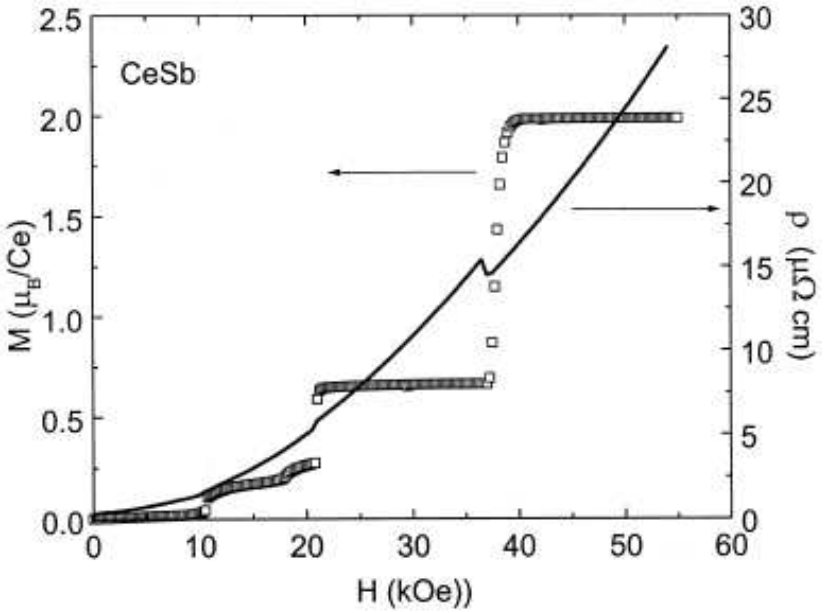

Fig. 4. Magnetization as a function of applied field (□, left-hand axis) and resistivity as a function of applied field (———, right-hand axis) at 5 K.

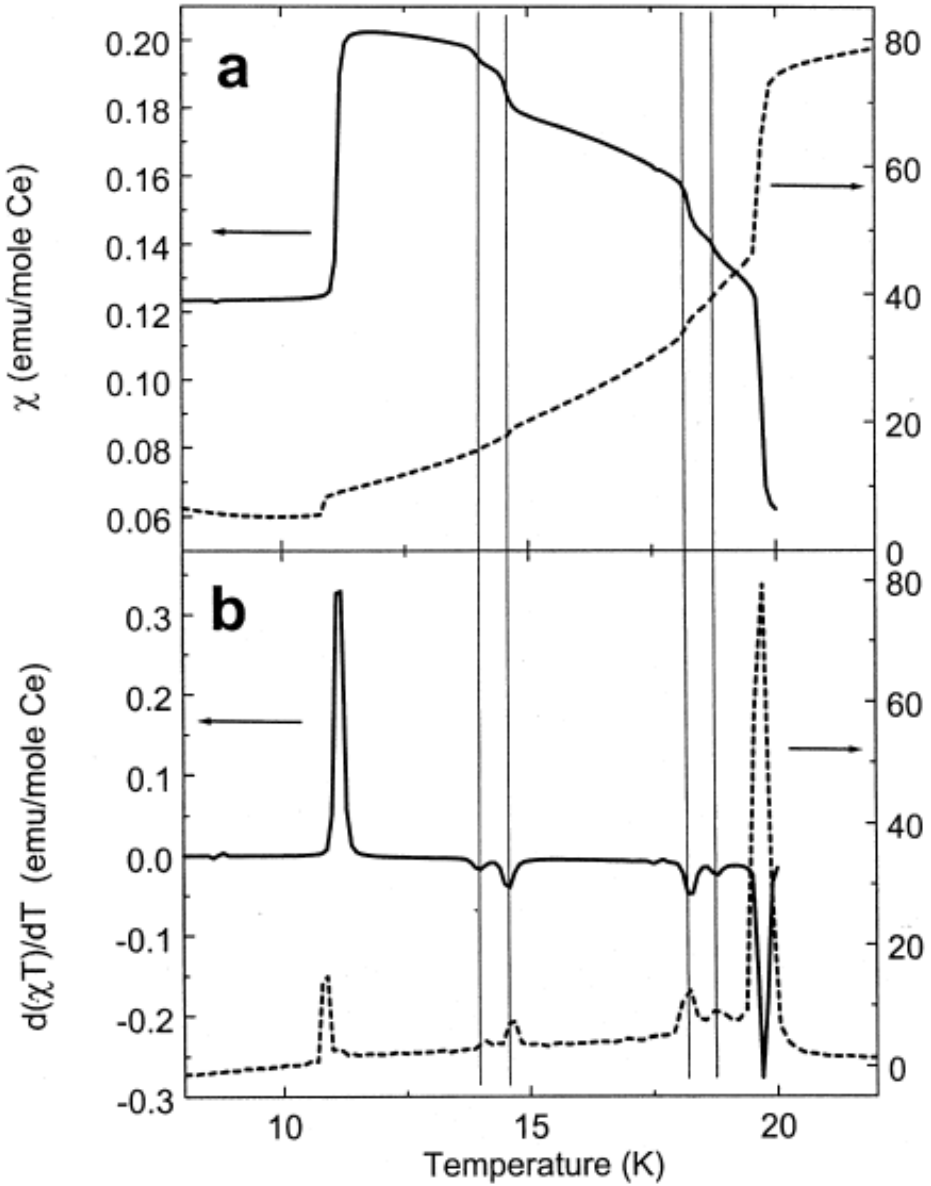

Fig. 6. (a) Dc susceptibility (———, left-hand axis) and resistivity (- - -, left-hand axis) as a function of temperature at 30 kOe. (b) $d(\chi T)/dT$ (———, left-hand axis) and $d\rho/dT$ (- - -, right-hand axis) at 30 kOe as a function of temperature. In both panels, vertical arrows highlight the boundaries of proposed new phases as described in text.

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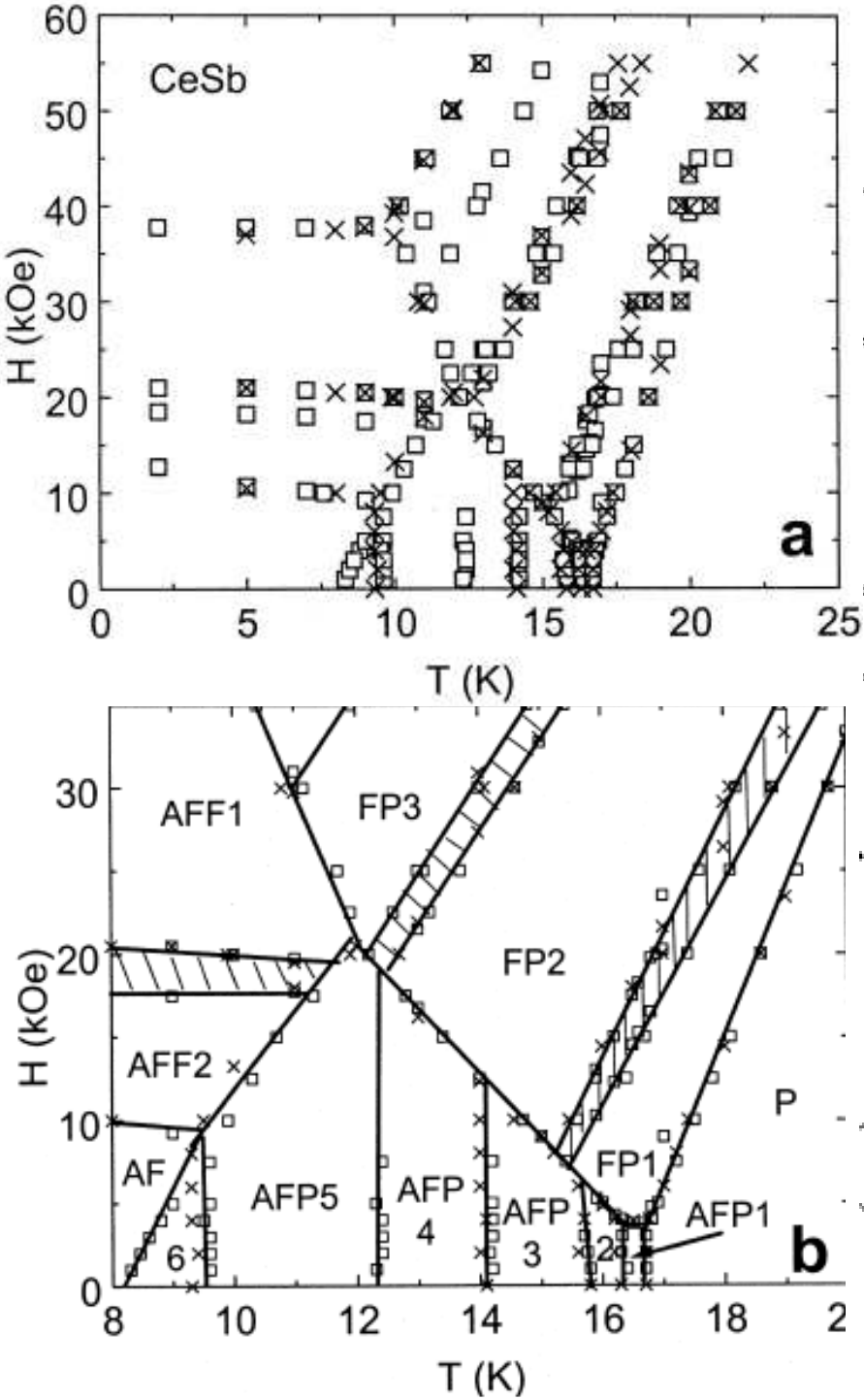
Multiple transitions in temperature and field

CeSb

M(H), M(T), ρ(H) and ρ(T) data can be used to assemble an H-T phase diagram of fantastic detail. This system was studied extensively in the 70's and 80's by several neutron scattering groups as well as serving as the inspiration for the ANNNI model. The precise origin of this complexity is still an open question.



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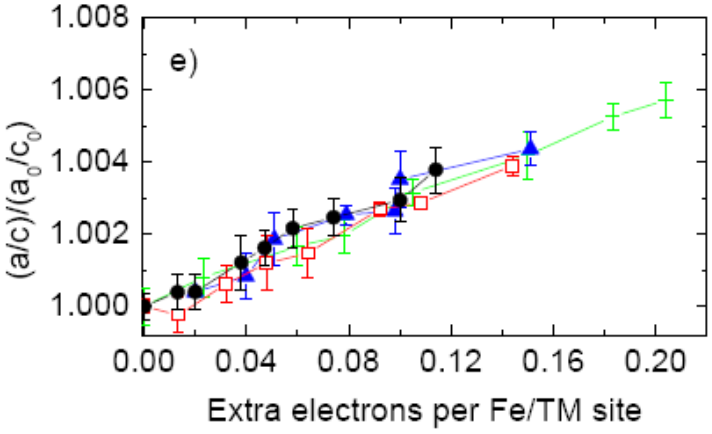
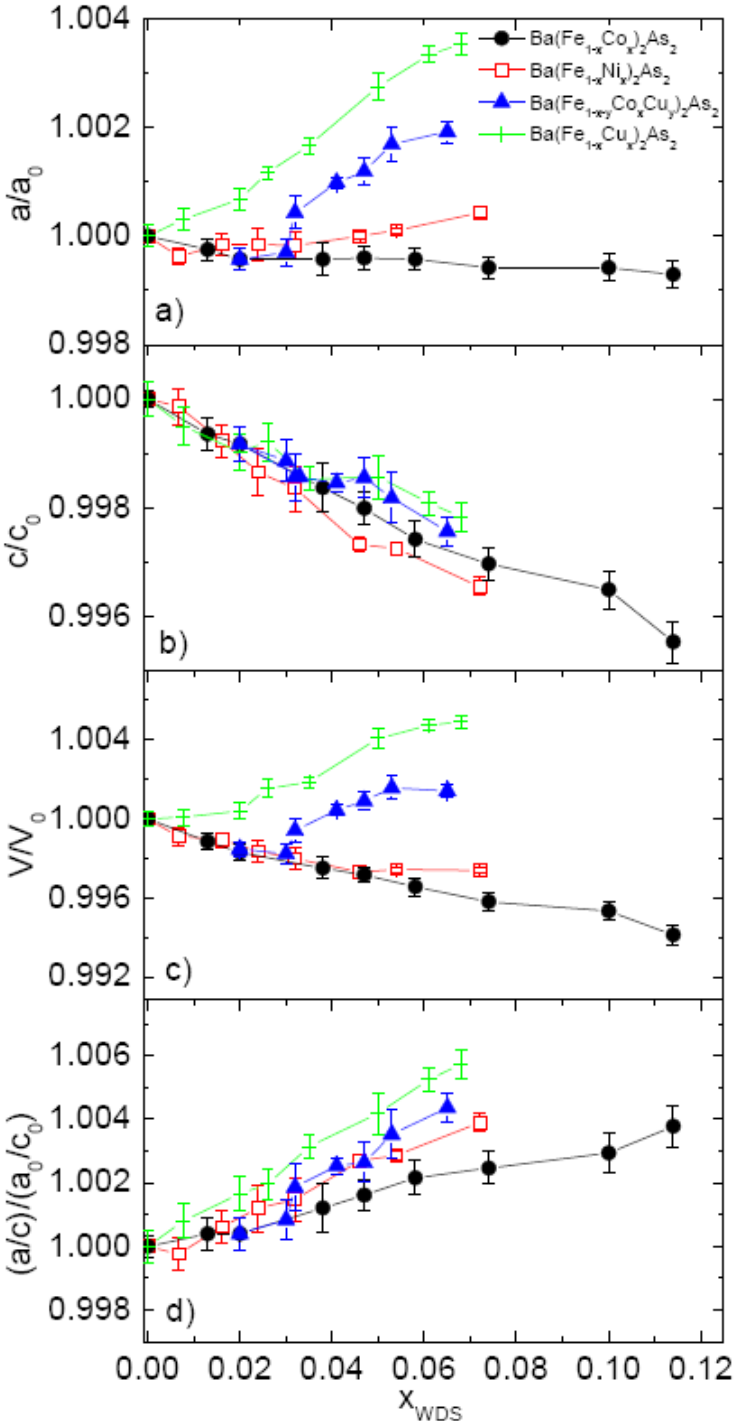
By substituting various TM for Fe in $BaFe_2As_2$ we change vary a number of different, but correlated, parameters.

x and e are not the only parameters that vary with doping: the lattice parameters change as well.

For 3d-TM doping, we find that c/c_0 varies as x and $(a/c)/(a_0/c_0)$ varies as e.

A key question is, "Can we separate x and e from the structural, c and a/c, parameters?





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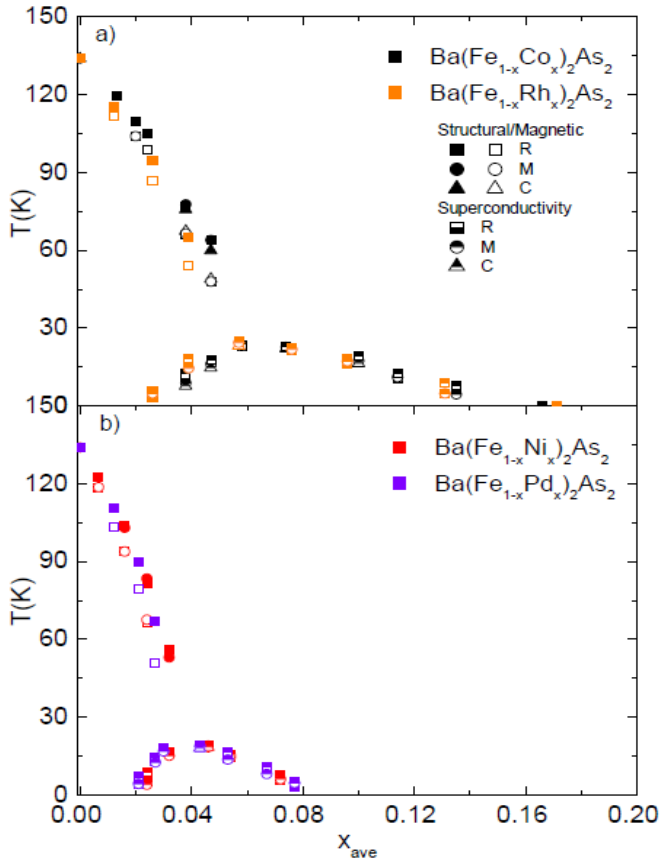
Although we find excellent scaling of the transitions with x and e, the changes in the lattice parameters (and their ratios) no longer parameterize the transitions for the 3d- and 4d-TM dopings. This can be seen in the plots of c/c_0 and $(a/c)/(a_0/c_0)$. The data group into 3d- and 4d- manifolds.

The upper phase transitions scale with a very local parameter: x.

The superconducting transition depends on e (band filling), at least on the over-doped side.



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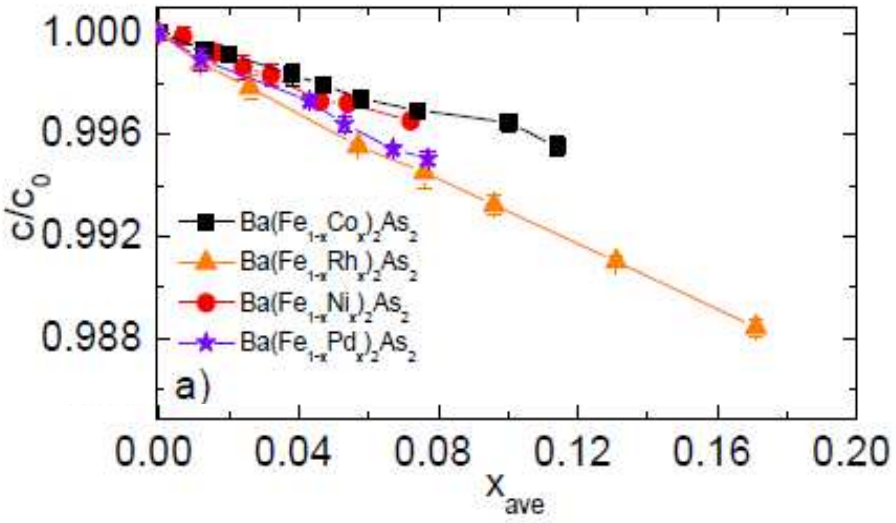
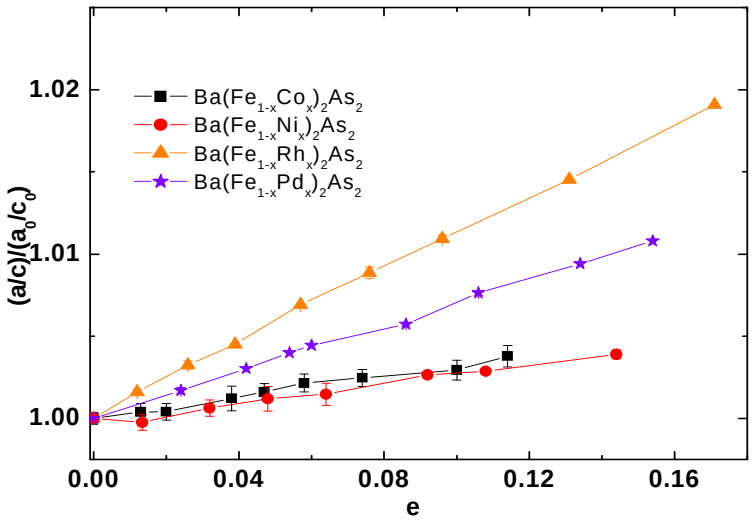
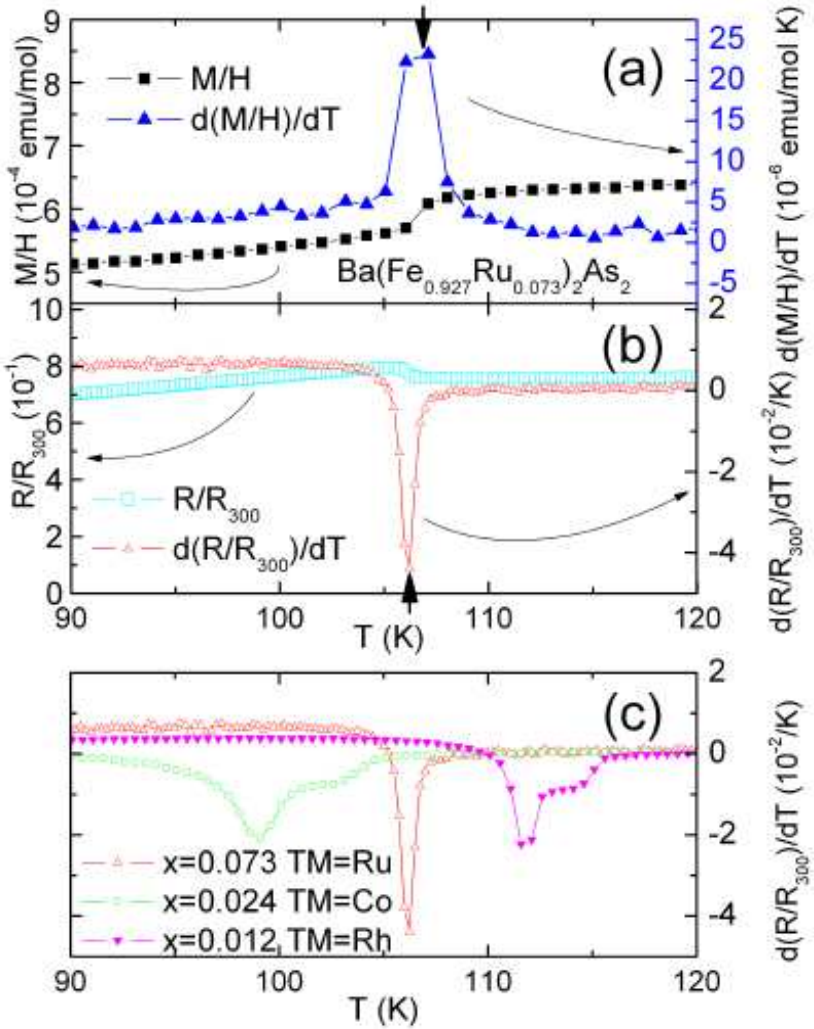
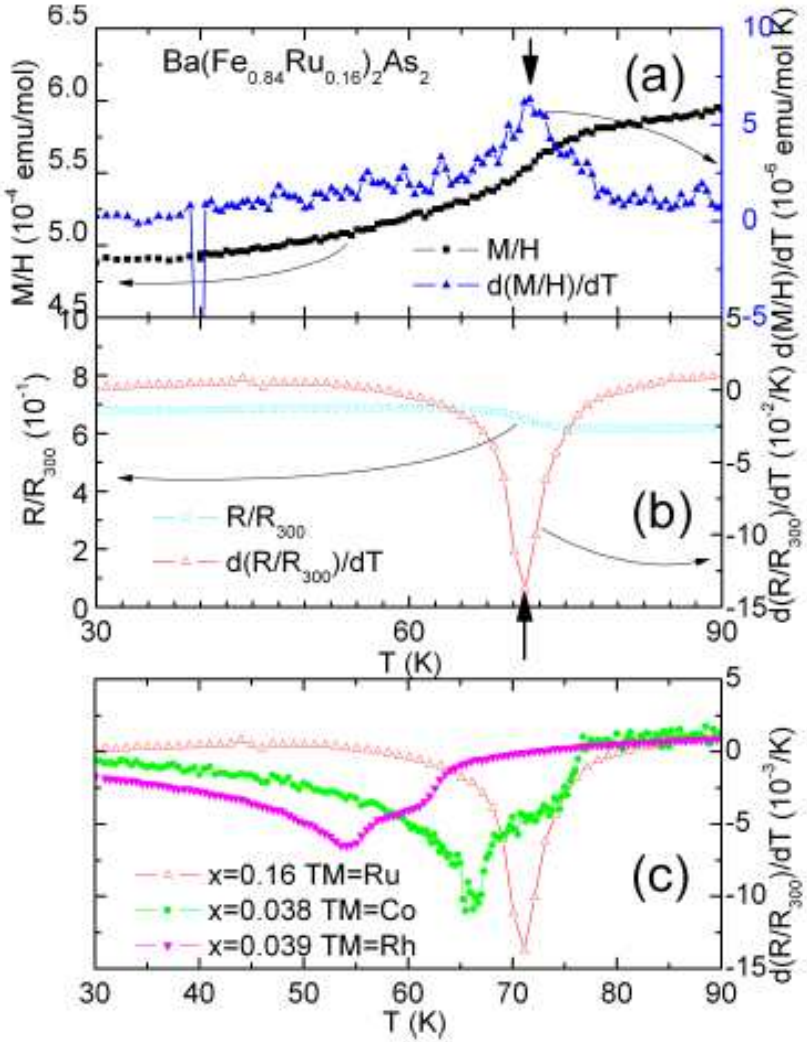





(a)
M/H
d(M/H)/dT
Ba(Fe0.927Ru0.073)2As2
M/H (10-4 emu/mol)
d(M/H)/dT (10-6 emu/mol K)
(b)
R/R300
d(R/R300)/dT
R/R300 (10-1)
d(R/R300)/dT (10-2/K)
T (K)
(c)
x=0.073 TM=Ru
x=0.024 TM=Co
x=0.012 TM=Rh
d(R/R300)/dT (10-2/K)
T (K)


Ba(Fe0.84Ru0.16)2As2
(a)
M/H
d(M/H)/dT
M/H (10-4 emu/mol)
d(M/H)/dT (10-6 emu/mol K)
(b)
R/R300
d(R/R300)/dT
R/R300 (10-1)
d(R/R300)/dT (10-2/K)
T (K)
(c)
x=0.16 TM=Ru
x=0.038 TM=Co
x=0.039 TM=Rh
d(R/R300)/dT (10-3/K)
T (K)