Higher T_c superconductivity: where we have found it, what we have done with it and where we should look for it.

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June 22, 2009

KITP

Workshop on Superconductivity

Ames Laboratory and Iowa State University

Mid-sized DOE Laboratory with ~ 400 employees organized in 1947 as result of Manhattan Project

Large land grant university (150 years old) with ~ 25,000 students. Known for Ag. (not Silver), Vet., and, in our circles, Physics and Chemistry associated with Ames Lab.

For 60 years Ames Laboratory / ISU has been a leader in the physics, chemistry and metallurgy of novel materials.

The past fourteen years have been an exciting time for intermetallic superconductors..

1994: RNi_2B_2C and YPd_2B_2C

2001: MgB_2

2008: $RFeAsO$ and $(AE)Fe_2As_2$

Each of these classes of compounds has pushed our understanding of superconductivity in intermetallic compounds, extending the range over which superconductivity is know to exist: to higher temperatures and new extremes of interaction with local moments as well as with the underlying lattice.

What can we learn from them, individually and as a whole?

The RNi_2B_2C compounds were poster children for the old prejudices of what made a good superconductor and why.

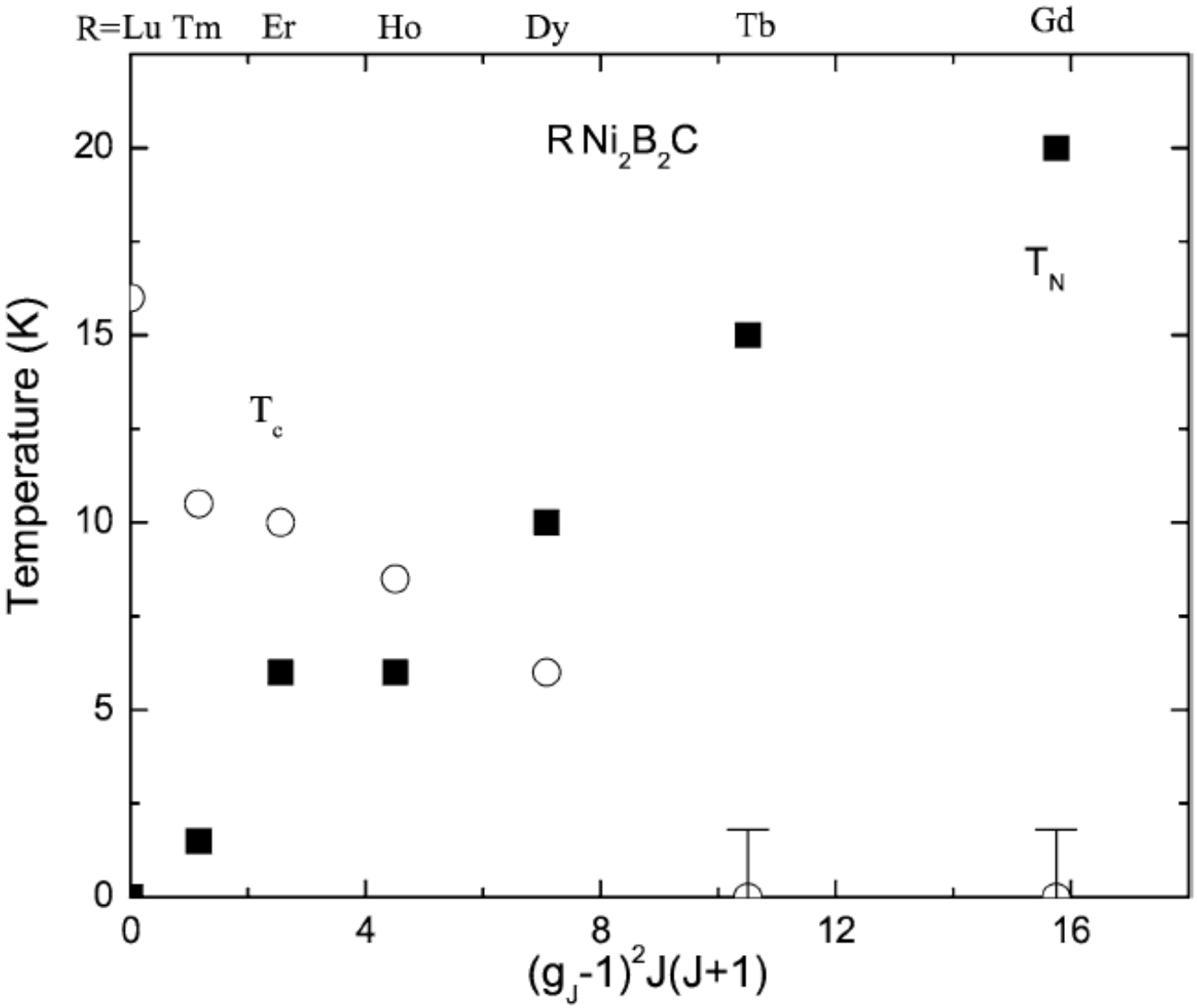
Light atoms / high characteristic frequencies
Strong electron phonon coupling, but no structural transition
Good $N(E_F)$, probably coming (in part) from transition metal

$LuNi_2B_2C$: T_C ~17 K
$N(E_F)$ large with significant Ni contribution
Very close to a structural phase transition
Large Debye temperature (high characteristic frequency)

YPd_2B_2C: T_C ~ 23 K
Metastable….If annealed loses structure---basically "just beyond" a structural phase transition, but, like diamond, can be trapped into structurally metastable state.

R. J. Cava *et al.*, Nature **367**, 146 (1994). R. J. Cava *et al.*, Nature **367**, 252 (1994). T. Siegrist *et al.*, Nature **367**, 254 (1994).

RNi_2B_2C family R = Gd – Lu, Y



Magnetic order for R = Gd, Tb, Dy, Ho, Er, Tm. T_N values ranging from 20 K to 1.5 K

Superconducting for R = Dy, Ho, Er, Tm, Lu, Y. T_C values ranging from 17 K – 6 K.

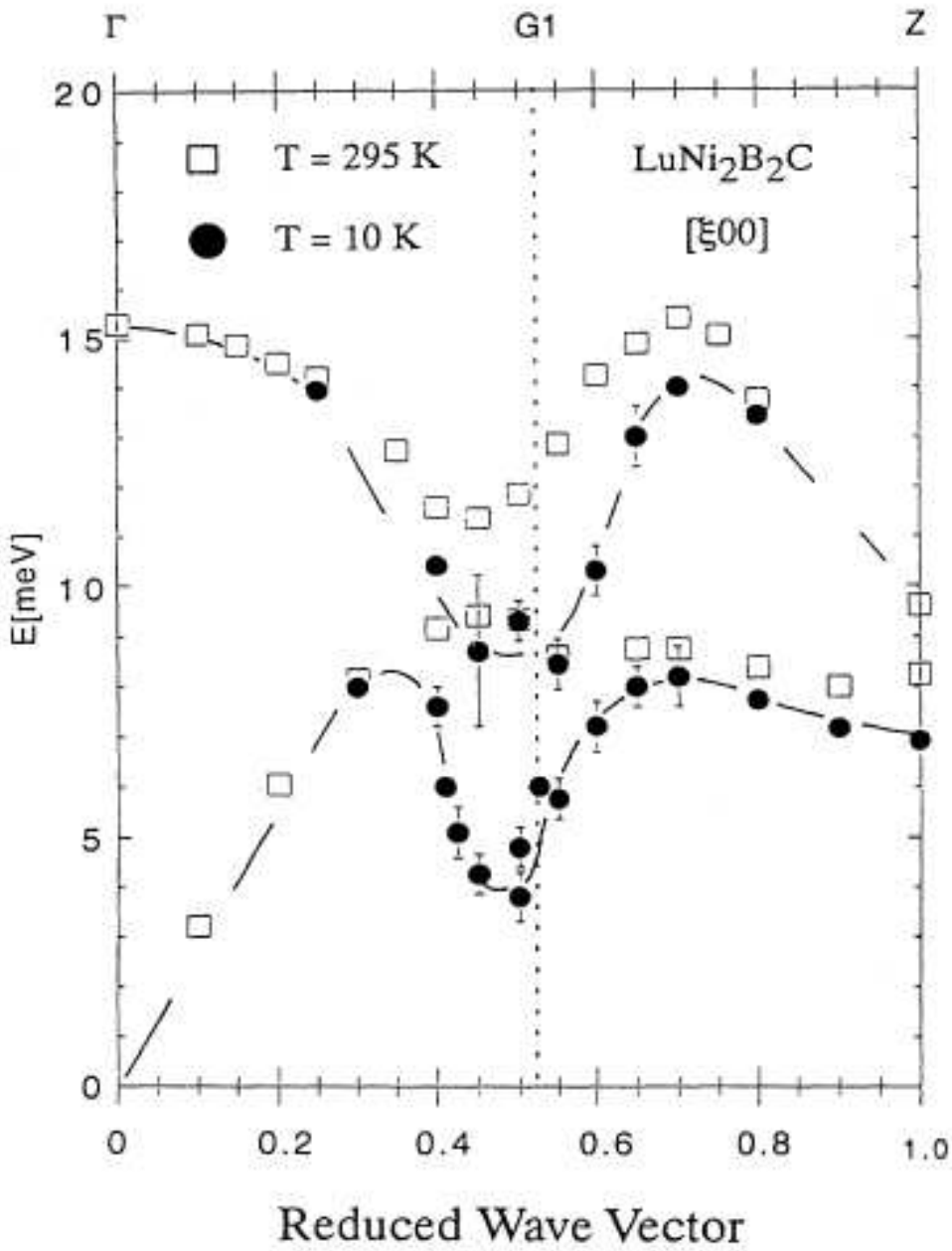
For R = Dy, Ho, Er, Tm there is strong interplay between the local moments and superconductivity. For $DyNi_2B_2C$ $T_N > T_c$, which is very rare for a local moment system.

P. Canfield et al. Physics Today Oct. 1998, 40.

$LuNi_2B_2C$ appears to be at the end of what electron – phonon coupling can offer. It appears to be at the hairy edge of a CDW instability.

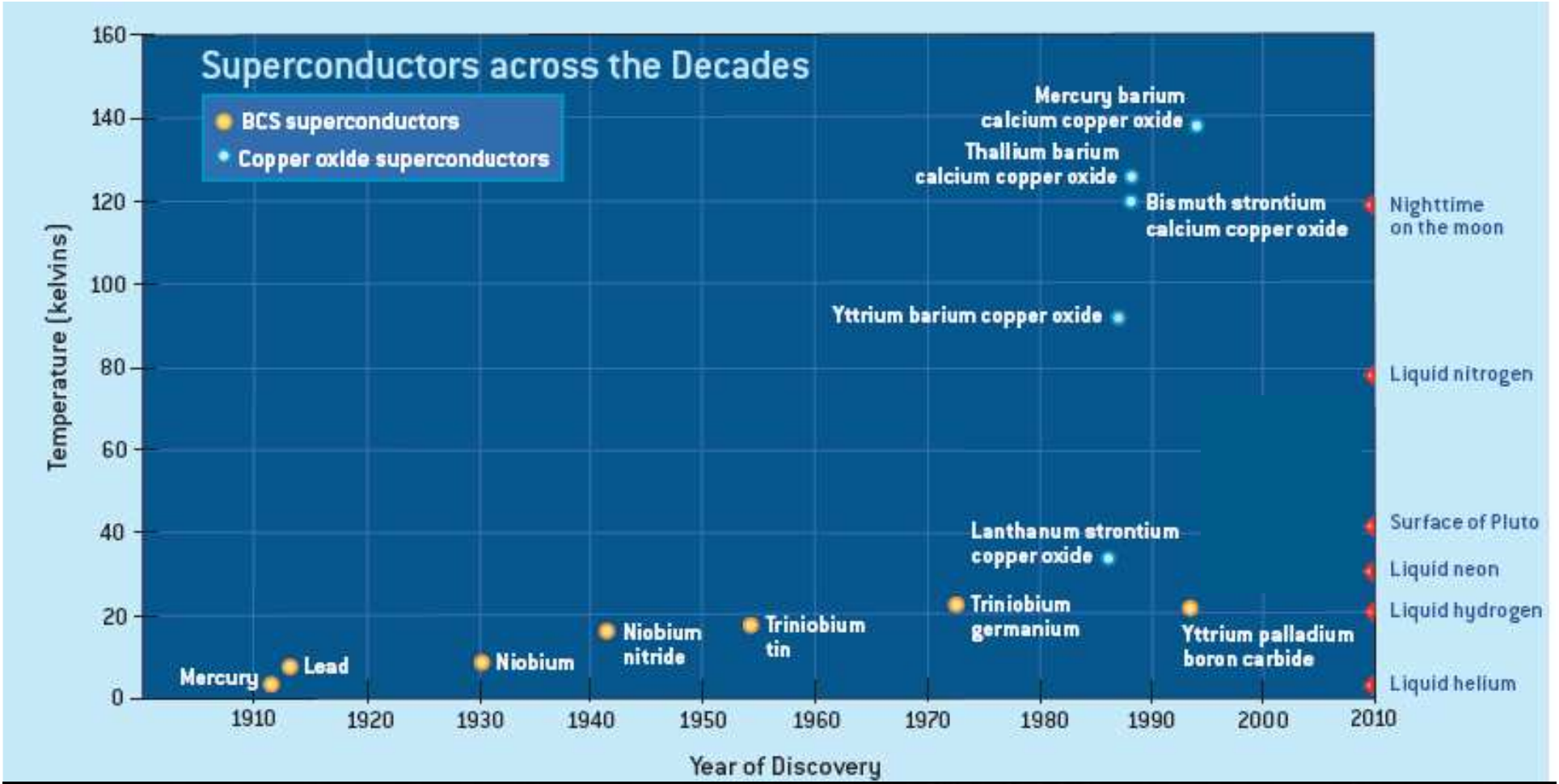
If the electron phonon coupling were increased further, then the phonon would soften further and there would be a structural phase transition…. This is consistent with the higher T_c and metastability of YPd_2B_2C .

Indeed all doping as well as pressure only suppress T_c in the RNi_2B_2C compounds.



Dervenagas et al. PRB **52** (1995) 9839

In terms of increasing T_c, YPd_2B_2C (and RNi_2B_2C) materials were a reminder that intermetallics were still promising…..



By PAUL C. CANFIELD AND SERGEY L. BUD'KO

In the late 1990's the question arose: "So, what to do next?"

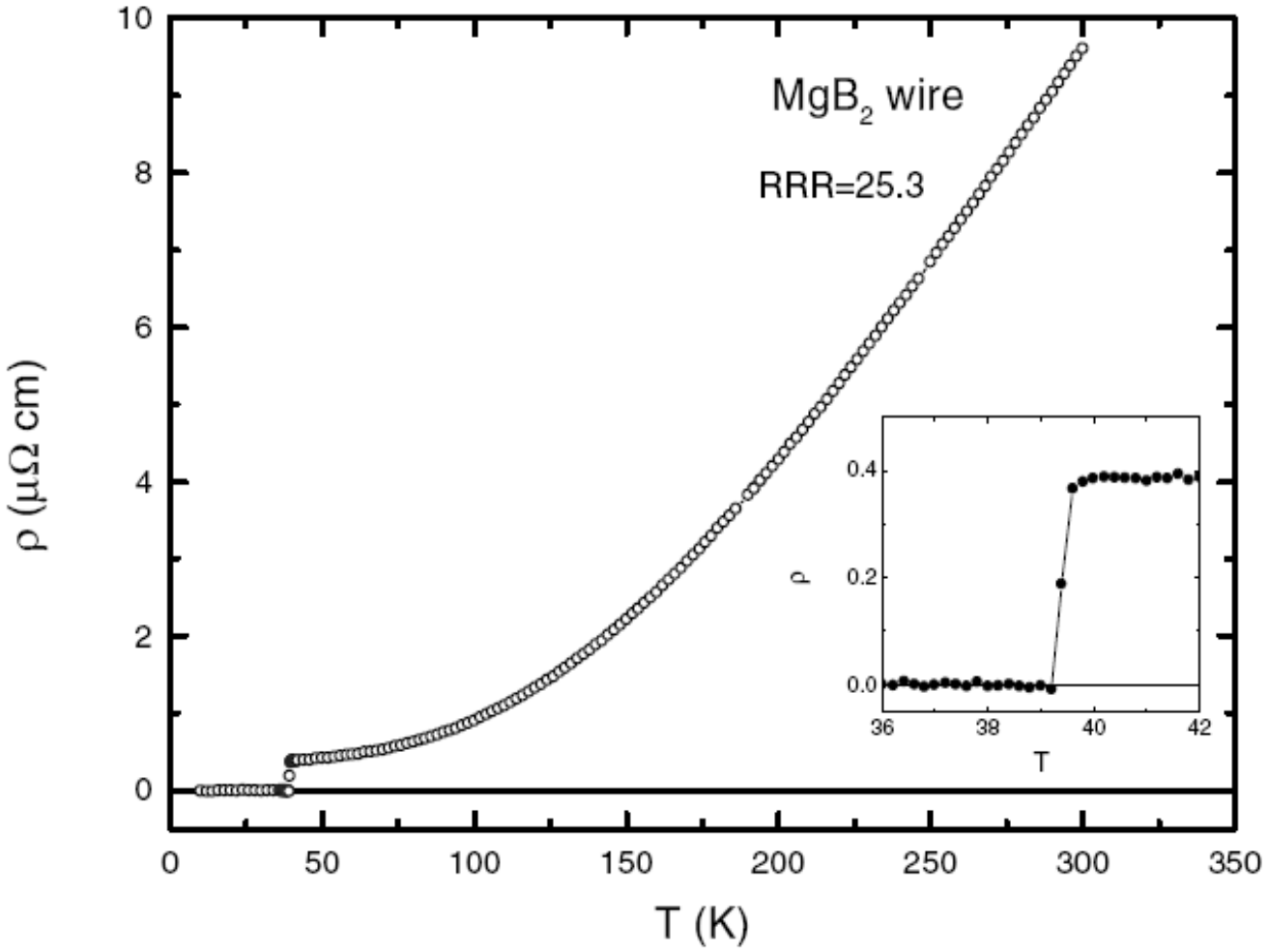
Based on the wealth of physics, as well as the high T_c values, found in the RNi_2B_2C family many groups decided to look for other intermetallics with light elements and see if similar (or even higher) T_c values could be found.

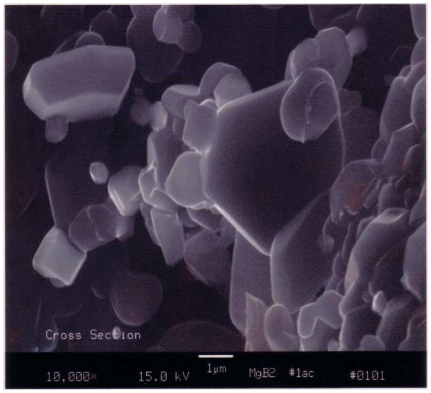
Several groups (including our Ames group) were examining compounds with combinations of Li, Be, B, C, Mg, Al, Si and other (often transition metal) elements.

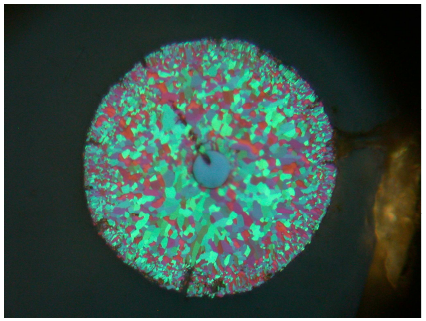
In late 2000 the group lead by Prof. J. Akimitsu examined the Ti-Mg-B ternary (*Ti because we got to have those 3-d electrons*) and found…a binary: MgB_2.

In mid-January, 2001 Prof. Akimitsu announced an ~40 K T_c in MgB_2 as part of a passing reference in a talk at a meeting….This started several groups to examining the compound.

We were able to devise a fast and efficient route for synthesis of high purity MgB_2 samples.







P.C. Canfield, D.K. Finnemore, S.L. Bud'ko, J.E. Ostenson, G. Lapertot,* C.E. Cunningham,† and C. Petrovic

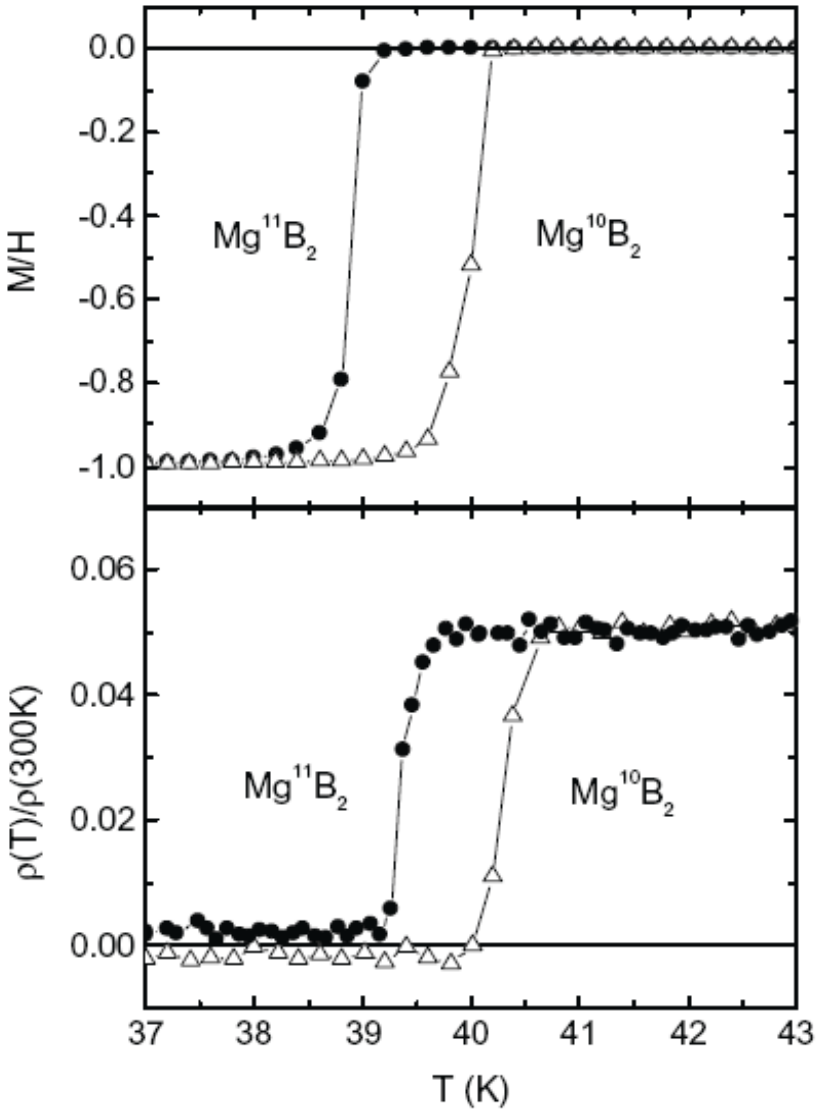
Boron Isotope Experiment

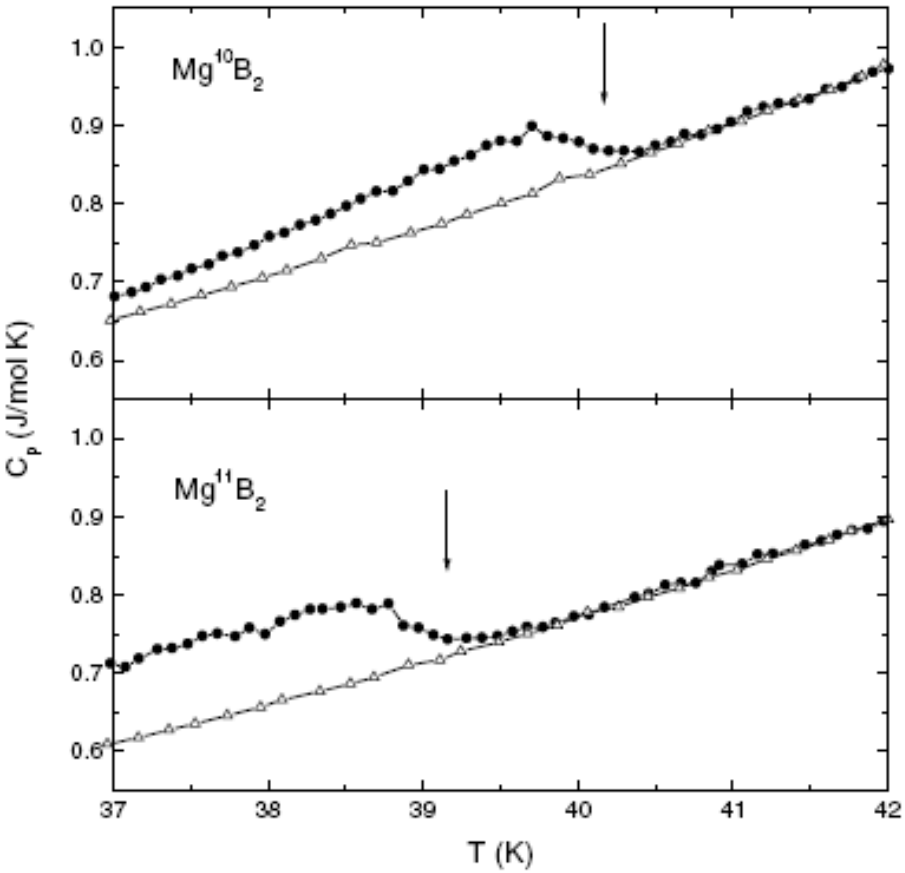
$\Delta T = 1.0$ K

(for simplest model expected $\Delta T_C \sim 0.85$)

$T_C \sim M^{\alpha_B}$, $\alpha_B = 0.26$

Consistent with phonon-mediated BCS.





VOLUME 86, NUMBER 9 PHYSICAL REVIEW LETTERS 26 FEBRUARY 2001

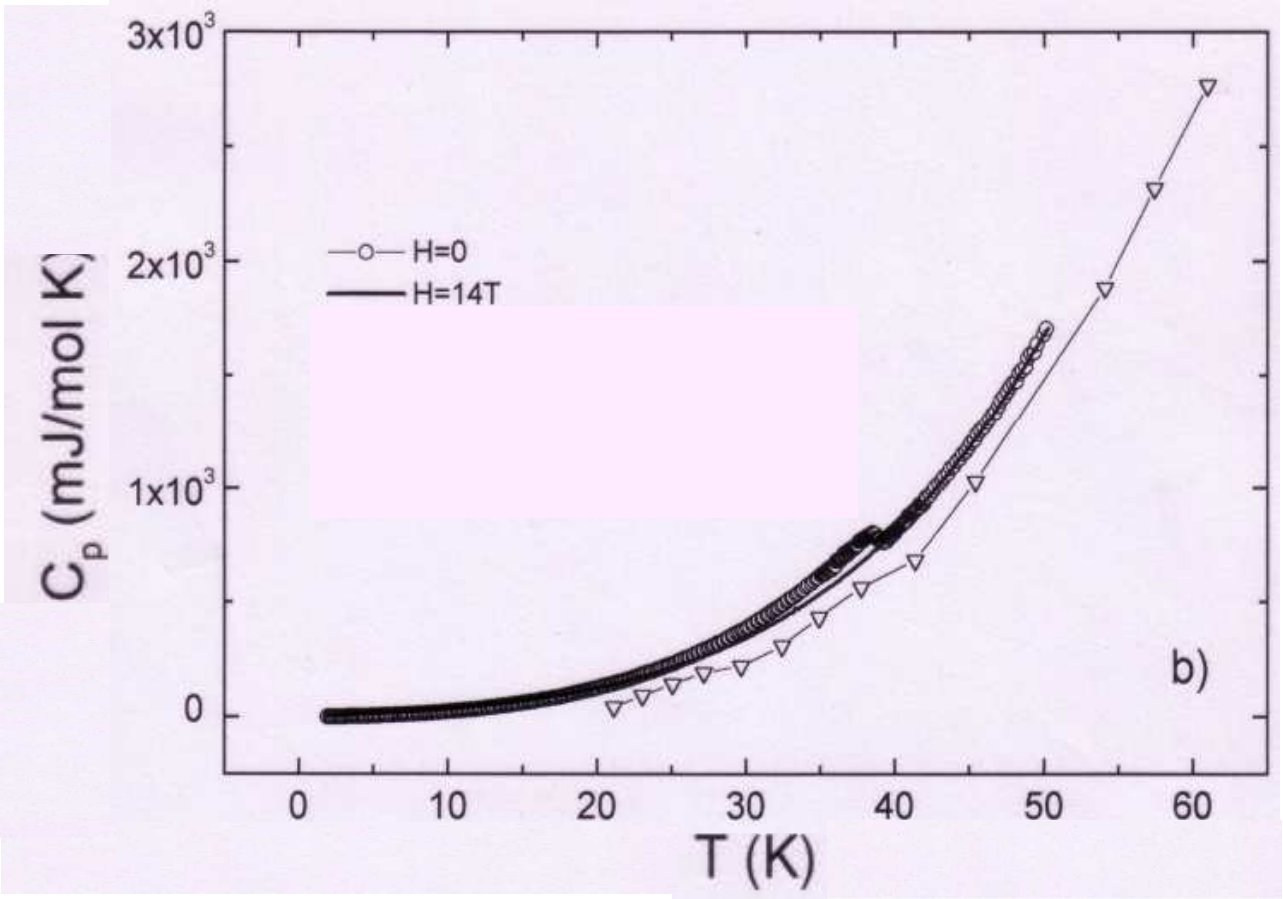
From $C_p(T)$ data we learn:

high ω_D for MgB_2…But,

$\gamma \sim 2.5 \pm 0.75$ mJ/mole-K^2

small γ, small $N(E_F)$)

	θ_D
For MgB_2	~ 750 K
For Mg	~ 320 K
For Si	~ 625 K
For Diamond	~1860 K



MgB_2 forces a shift in emphasis when looking for other higher T_C compounds

$$k_B T_C = 1.13 \hbar \omega_D e^{-1/VN(E_F)}$$

Old prejudice: Need to have large ω_D and large $N(E_F)$ and hope for good V

But MgB_2 has a very small $N(E_F)$ ($\gamma \sim 2.5$ mJ/mole-K^2)

So, MgB_2 is a low $N(E_F)$ superconductor

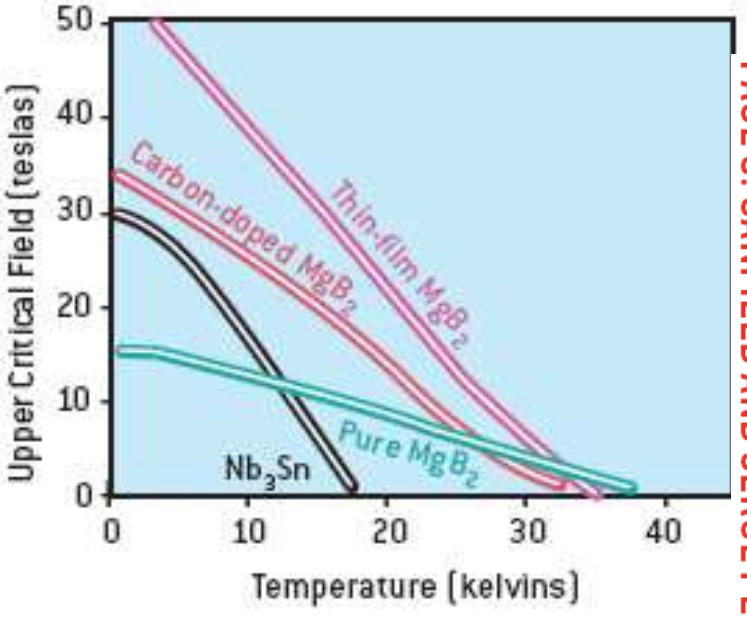
For searches for MgB_2 like compounds we should look for large ω_D and large V and not obsess about $N(E_F)$ so much….

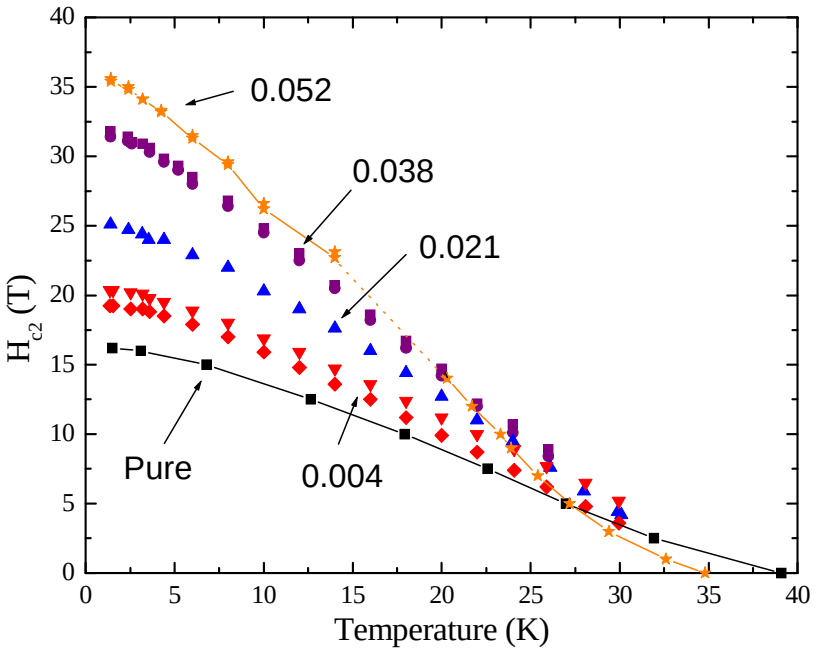
This is a much harder search algorithm.

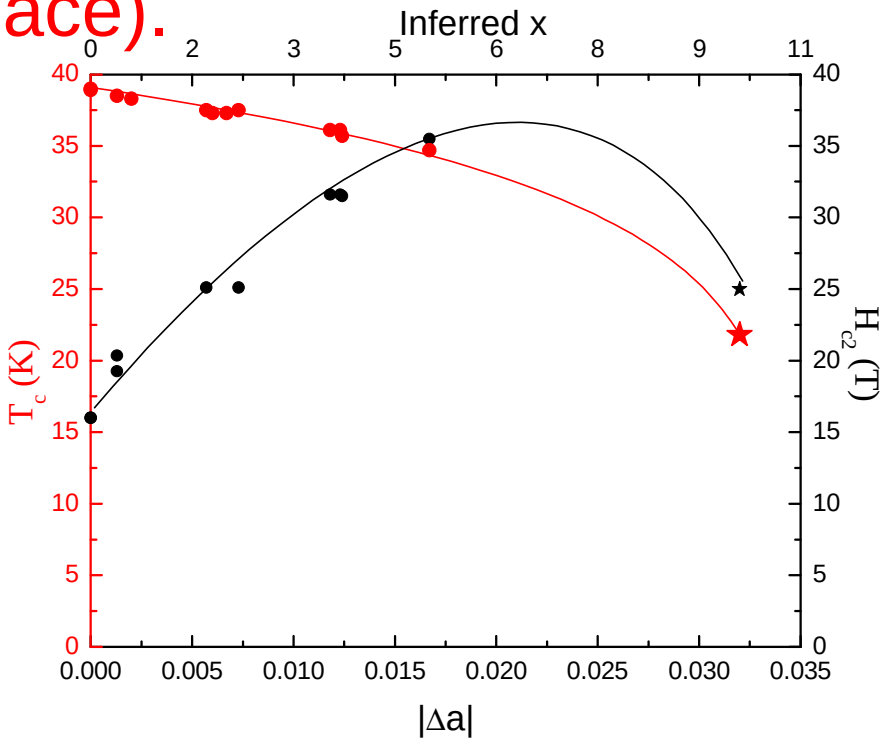
Given its T_c, there was a clear drive to see if MgB_2 could become a practical superconductor

$Mg(B_{1-x}C_x)_2$ studies

Tuning of T_C and H_{C2} with light carbon doping makes MgB_2 superior to Nb_3Sn (in H-T space).



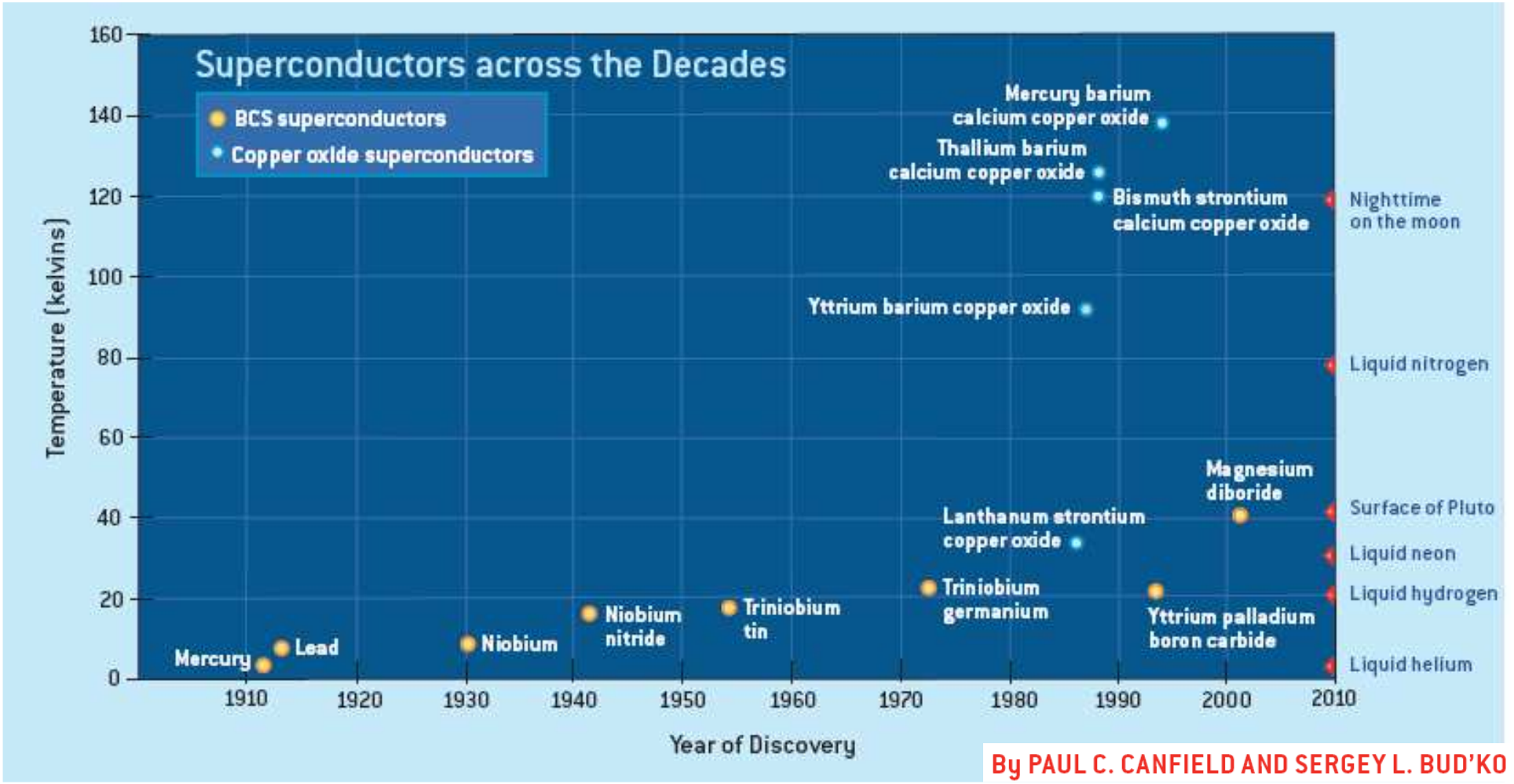




Phys. Rev. Lett. 92, 217003 (2004)

PAUL C. CANFIELD AND SERGEY L. BUD'KO SCIENTIFIC AMERICAN APRIL 2005 81

We were able to improve the superconducting properties of MgB_2 by judicious doping (H_{c2}) and control of grain size (J_c), but like the RNi_2B_2C materials any perturbation (doping, pressure) reduced T_c.



More recently, between February and May of 2008 two related classes of FeAs based compounds were found to superconduct.

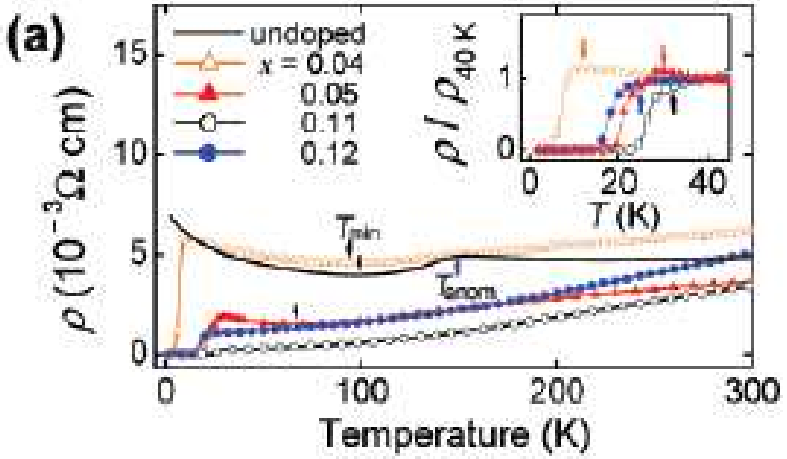
These compounds have T_c values that span from ~ 30 K to over 55 K; they appear to be part of a diverse and varied set of FeAs based materials and show early promise of being "user friendly" in terms of their superconductivity, although they are unfriendly in terms of arsenic….

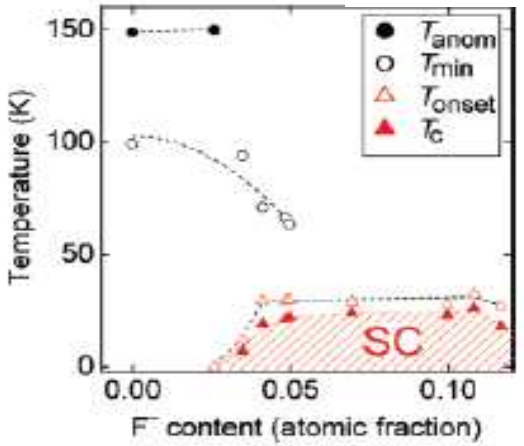
Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

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

J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

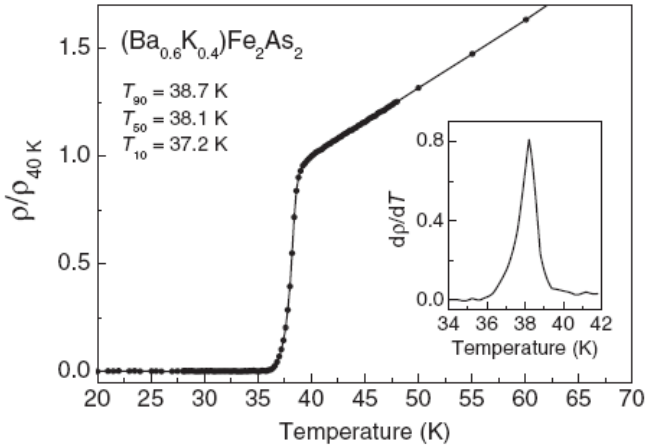




Superconductivity at 38 K in the Iron Arsenide $(Ba_{1-x}K_x)Fe_2As_2$

(Received 29 May 2008; published 5 September 2008)

Marianne Rotter, Marcus Tegel, and Dirk Johrendt*



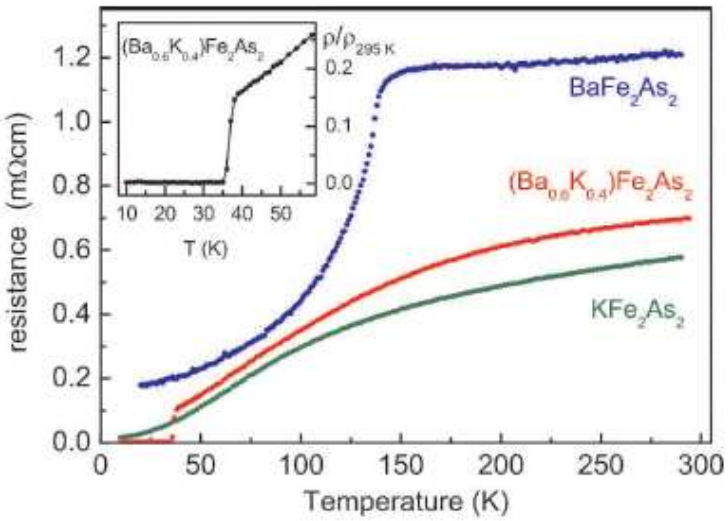
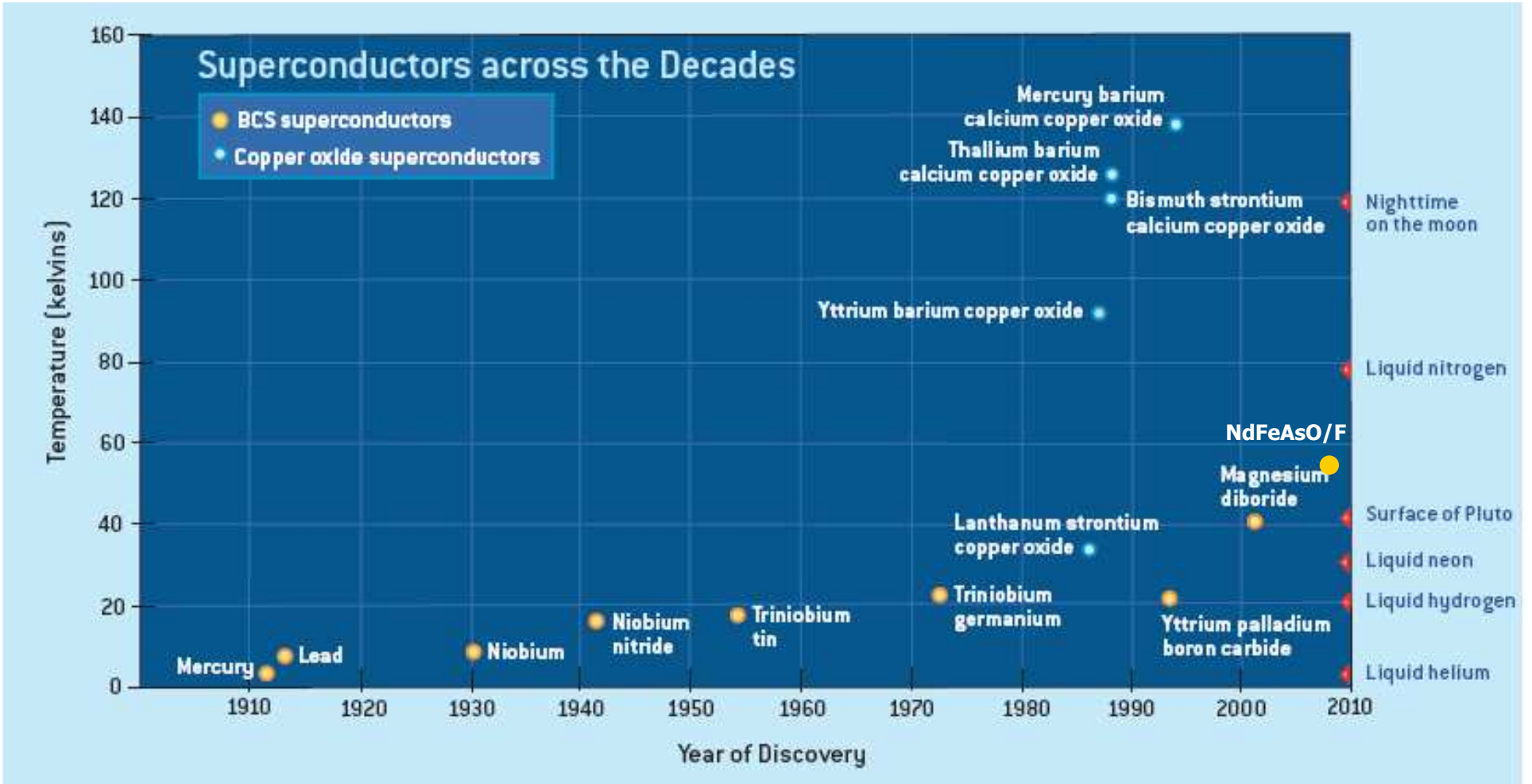


FIG. 4. Resistivity transition of $(Ba_{0.6}K_{0.4})Fe_2As_2$.

Updating our plot we see that T_c for these materials can be as much as ~15 K higher than MgB_2.

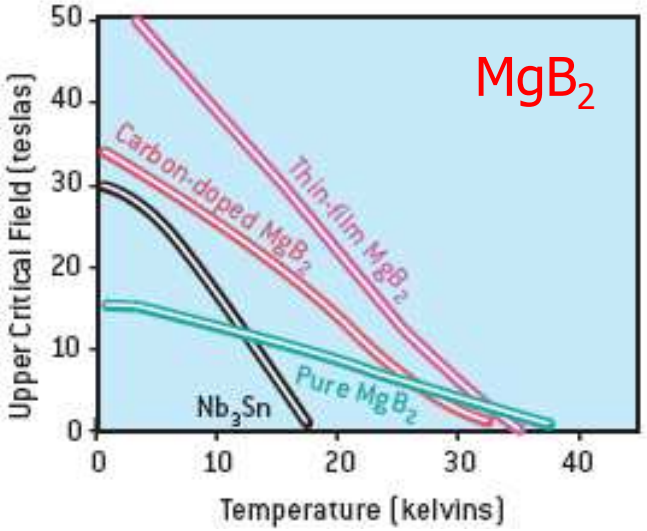
But what can we learn about them?



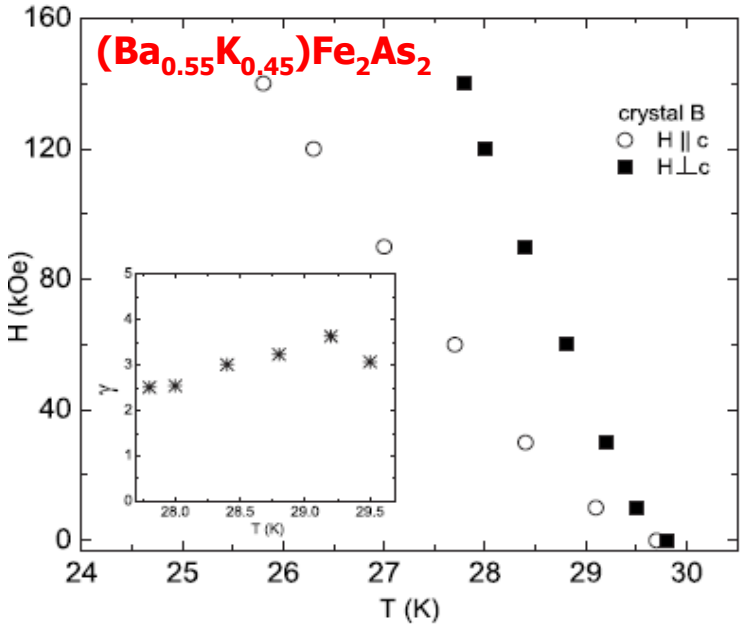
By PAUL C. CANFIELD AND SERGEY L. BUD'KO

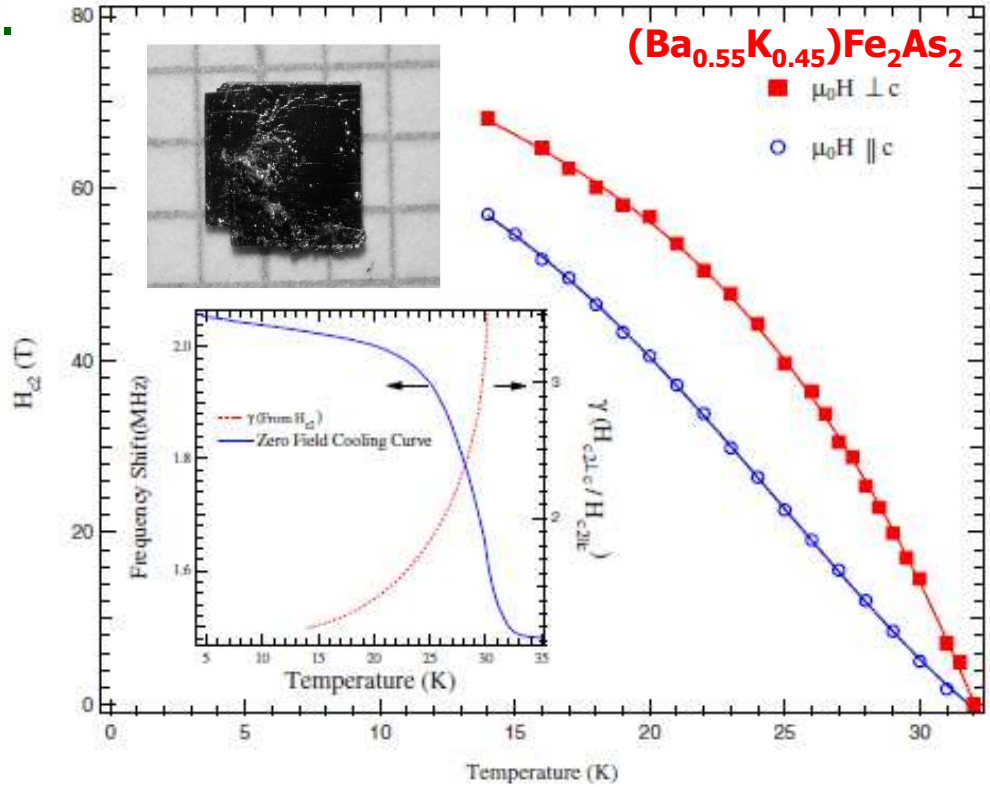
Single crystals of the $AEFe_2As_2$ (AE = Ba, Sr, Ca) compounds can be grown out of Sn and FeAs readily.

Anisotropic $H_{c2}(T)$ data indicate that FeAs compounds may well be of practical as well as basic interest.



ALTARAWNEH *et al.* PHYSICAL REVIEW B 78, 220505(R) (2008)





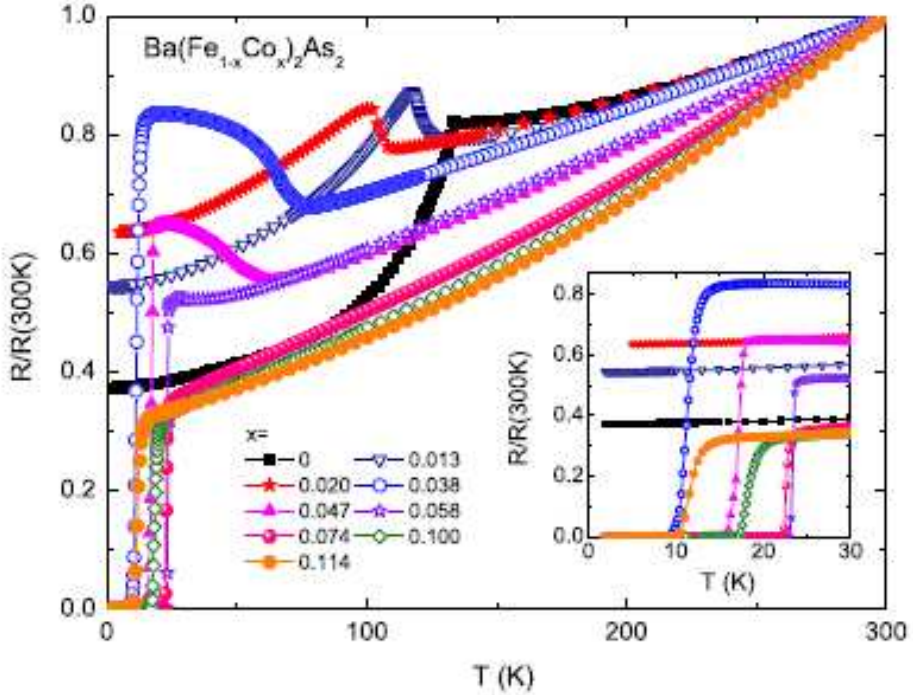
NI *et al.* PHYSICAL REVIEW B 78, 014507 (2008)

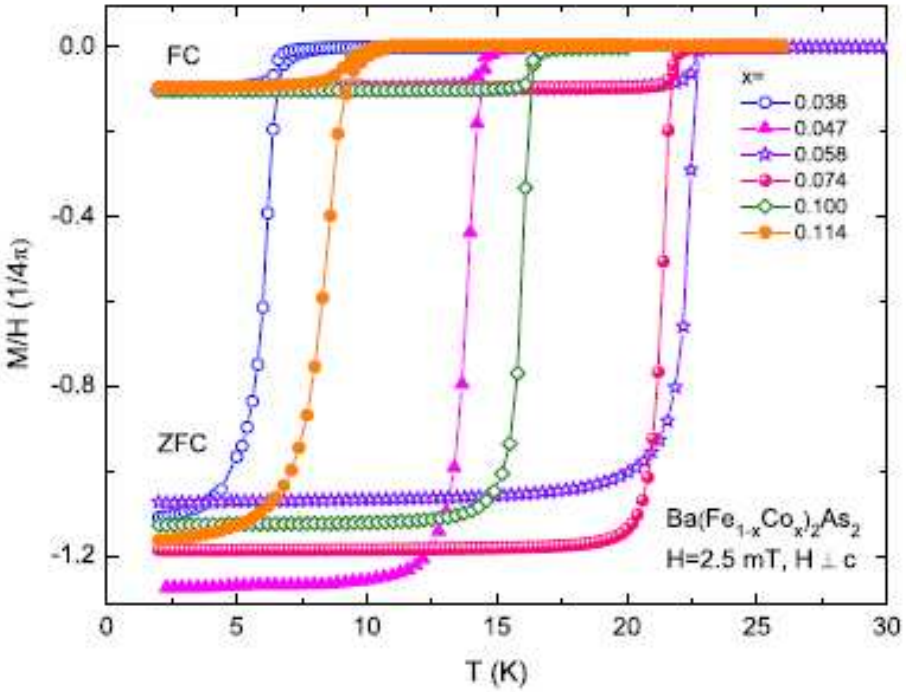
PHYSICAL REVIEW B 78, 214515 (2008)

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)



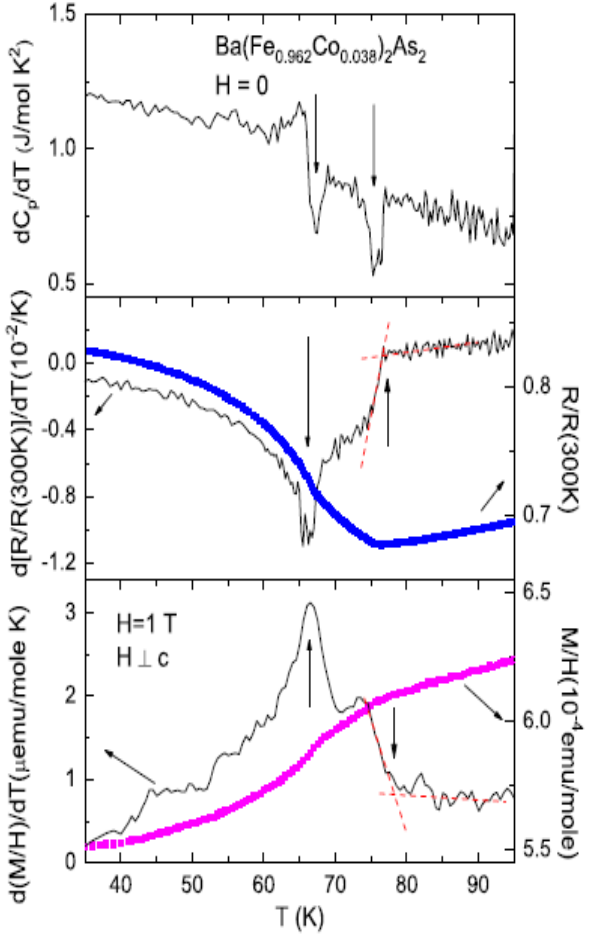


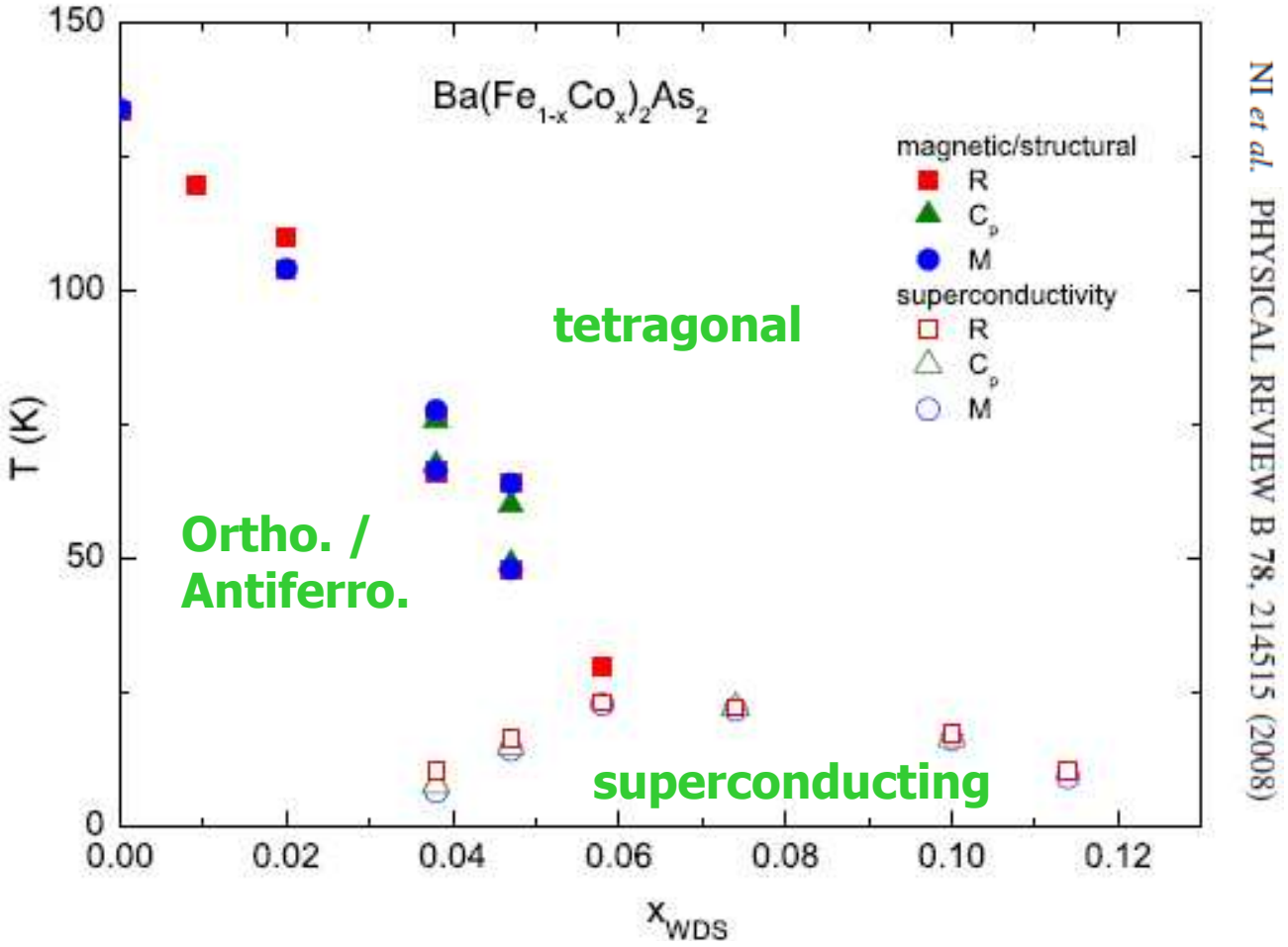
Doping of $AEFe_2As_2$ compounds on the Fe site with transition metals (TM) is also possible and important for two basically different reasons: (i) very different from CuO-based superconductors, (ii) offered easier and more homogeneous doping than K- or other alkali-doping.

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. Similar results were posted soon after by Fisher's group:

Jiun-Haw Chu
PHYSICAL REVIEW B 79, 014506 (2009)

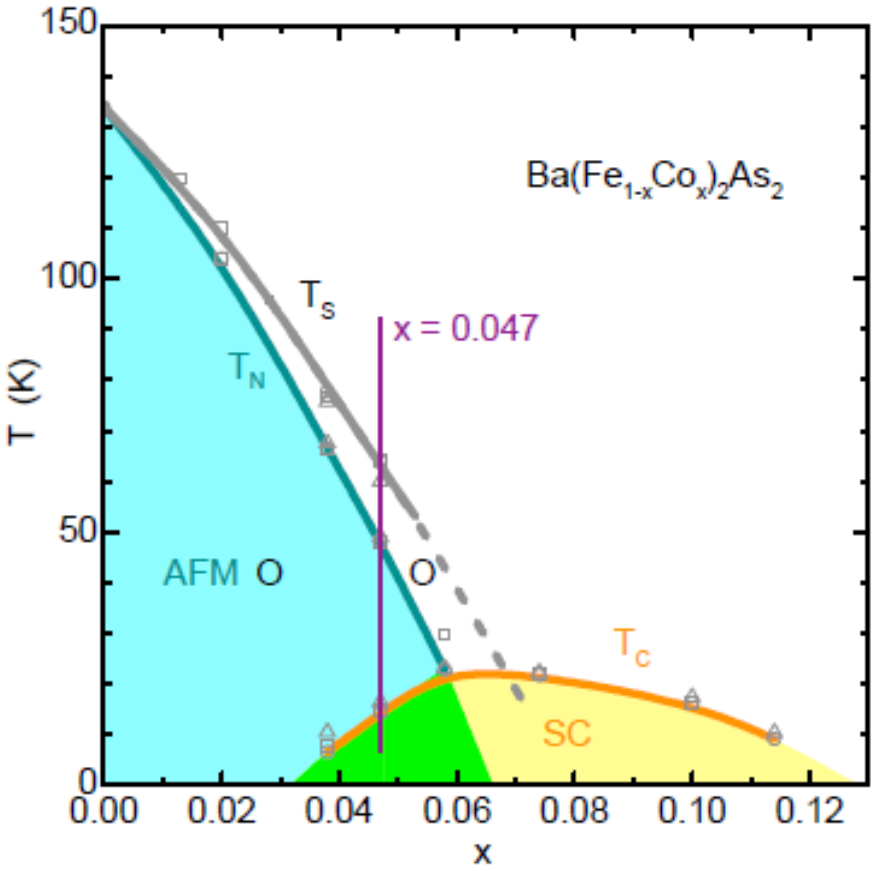
To clarify point (ii) microscopic data was needed….

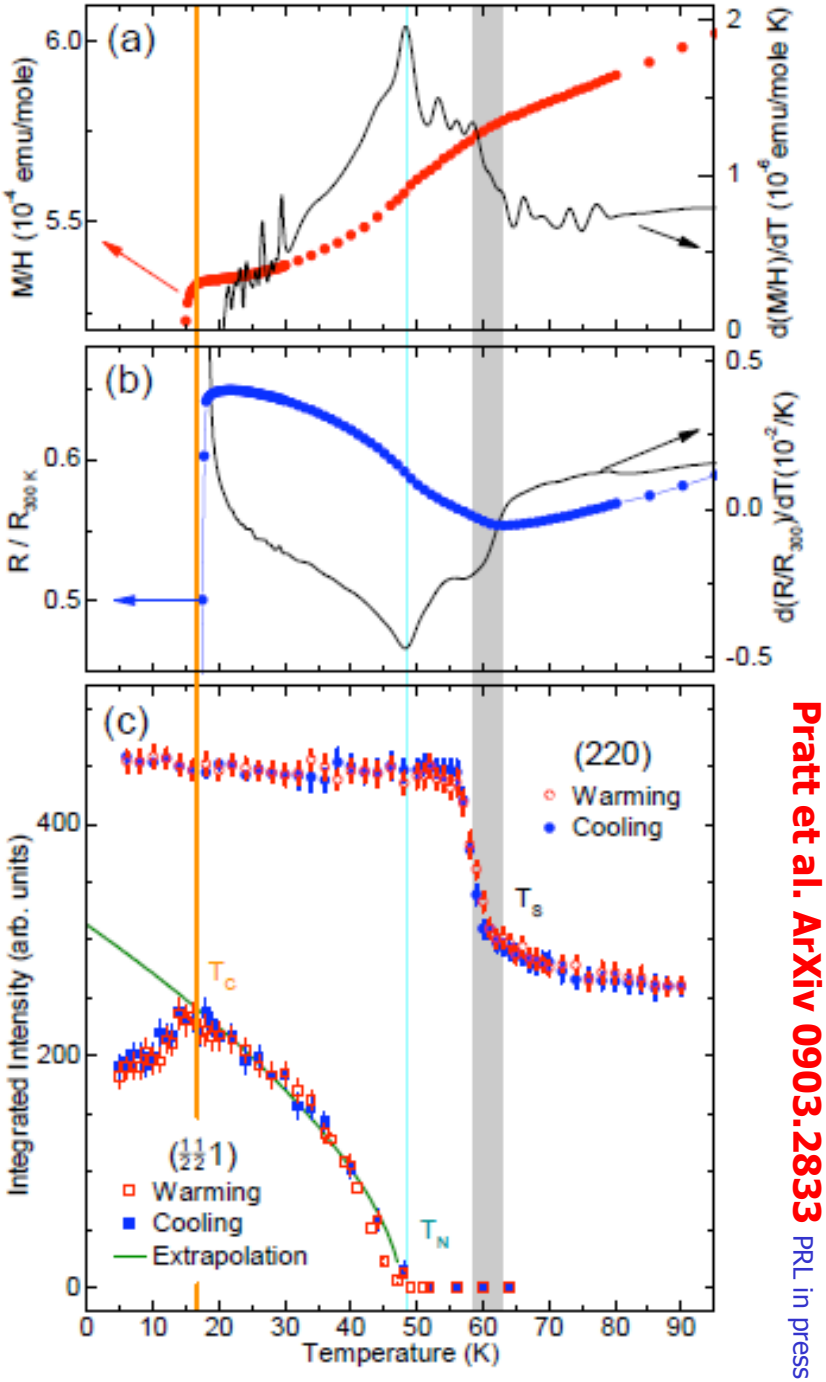




NI *et al.* PHYSICAL REVIEW B 78, 214515 (2008)

Neutron and X-ray scattering clarified the question of splitting / 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. ArXiv 0903.2833 PRL in press

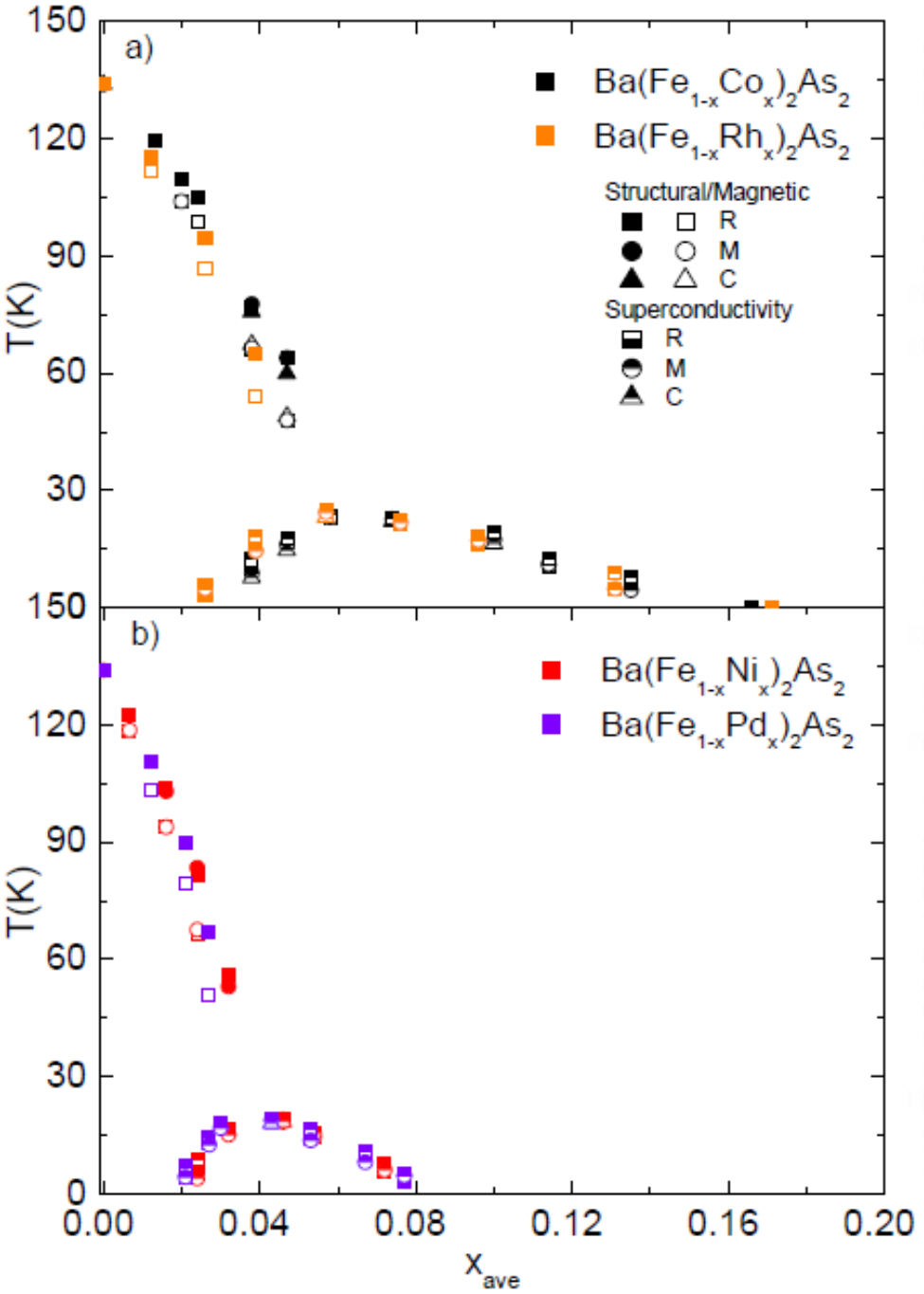
We have studied several electron doped TM substitutions: Co, Ni, Rh, Pd, etc.

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

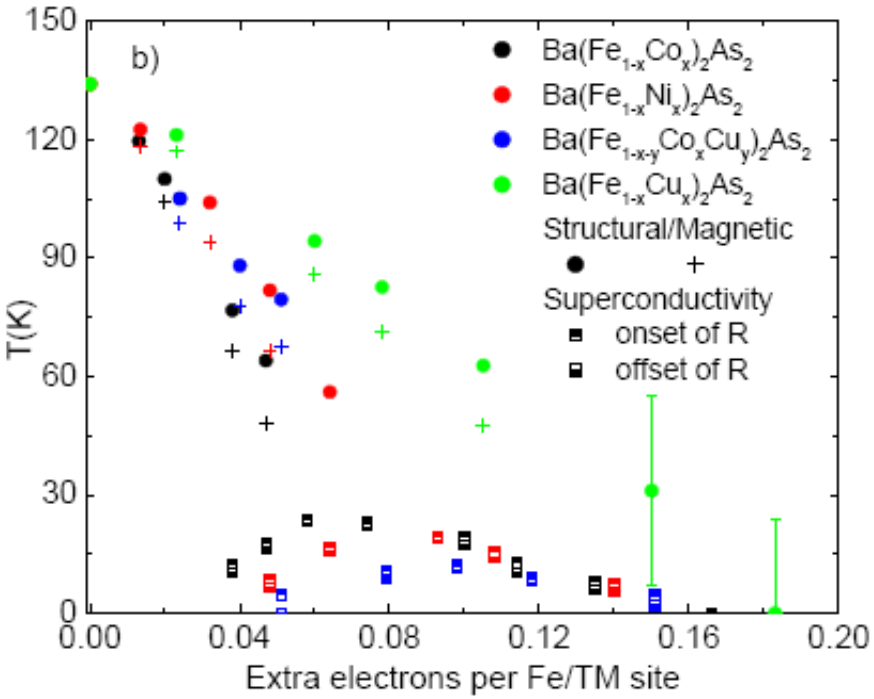
When we compare the isoelectronic Co- and Rh-doped series we find identical phase diagrams.

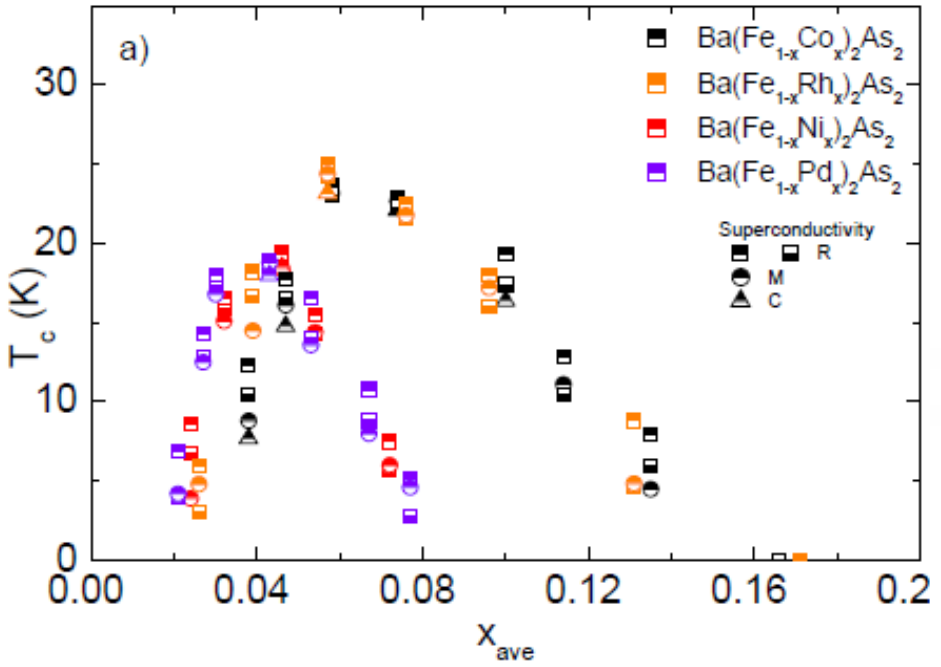
When we compare the isoelectronic Ni- and Pd-doped series we again find identical phase diagrams.

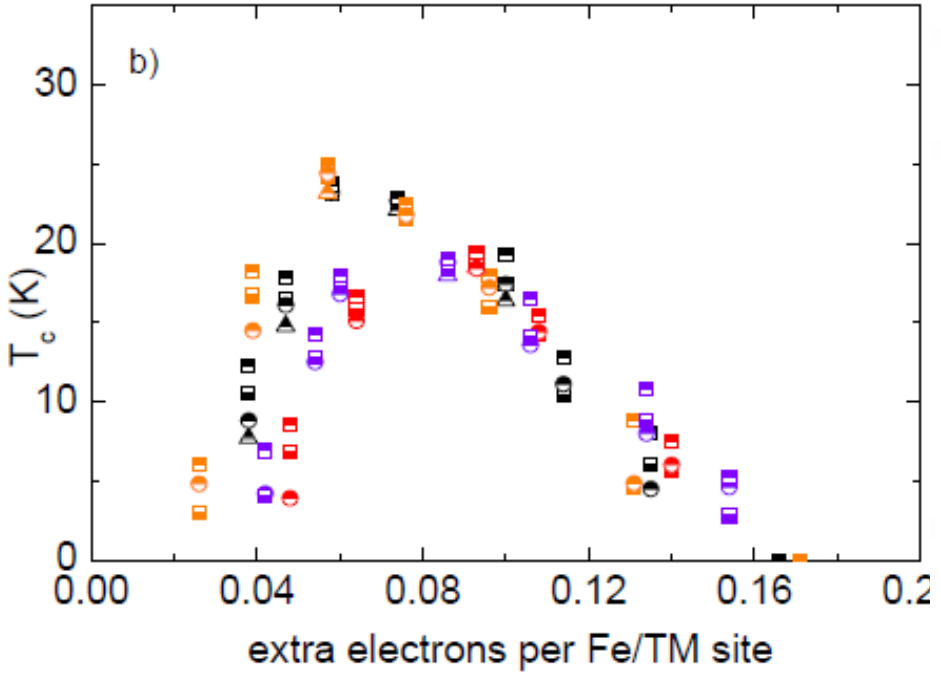
This remarkable similarity between the isoelectronic phase diagrams can only be appreciated if the actual x is determined. Nominal x-values differ from TM to TM' series.

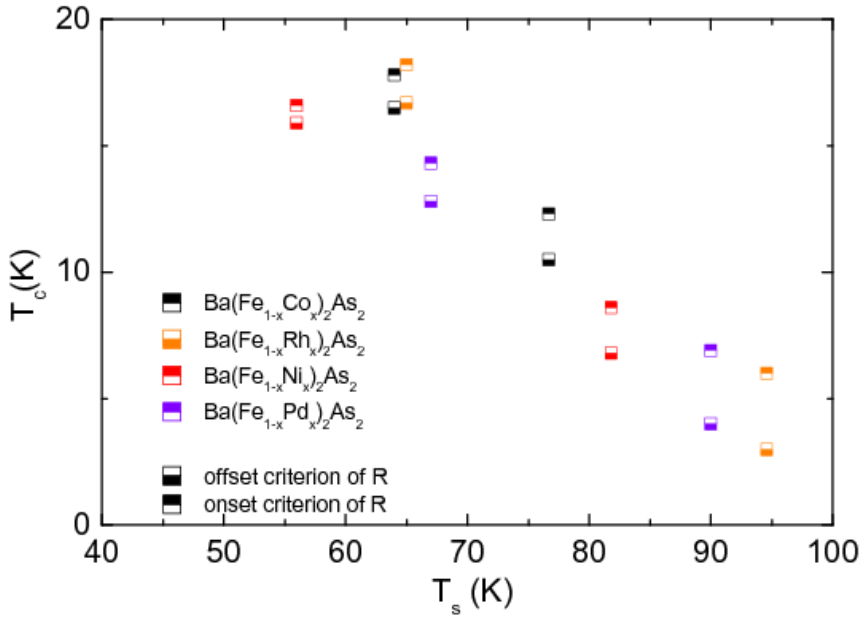


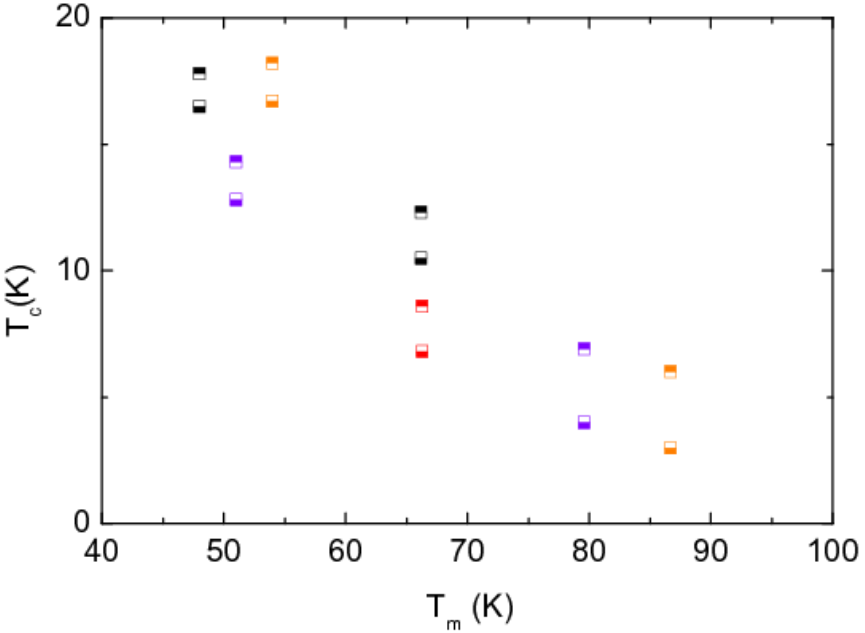
We can now examine the T_c dome in greater detail. There is excellent scaling of T_c with e on the over doped side. On the under-doped side, there is a variation that is associated with how far we have suppressed the upper transitions.





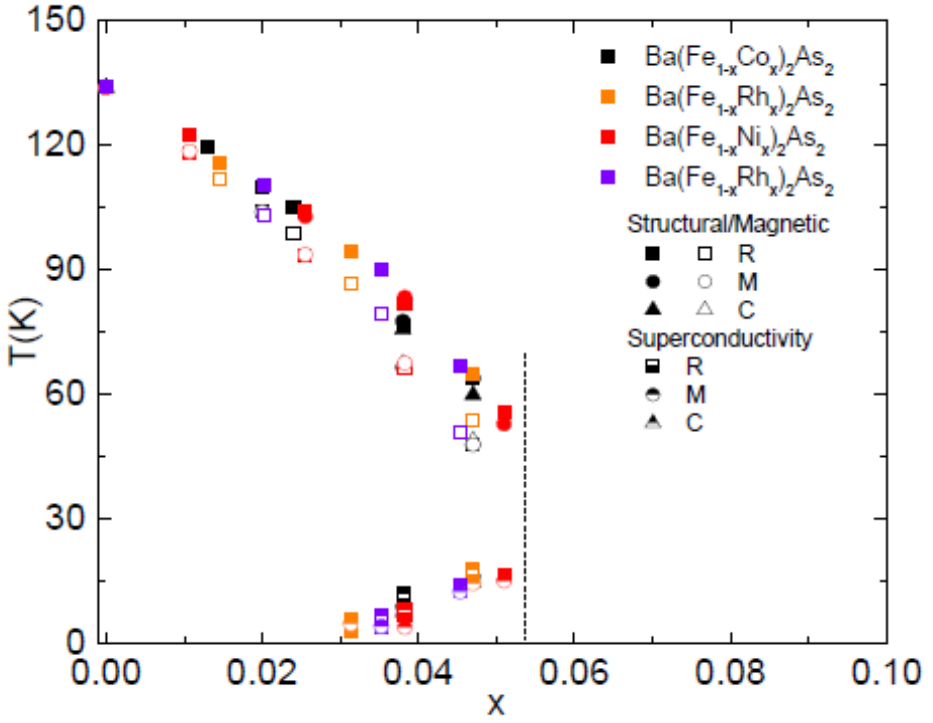






We can test this idea more quantitatively. Since there is a rough scaling between the upper transitions and x, perhaps the $T_c(x)$ scaling simply reflects the dependence of T_c on the value of the upper transition temperatures.

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



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 (band filling) that supports superconductivity 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.

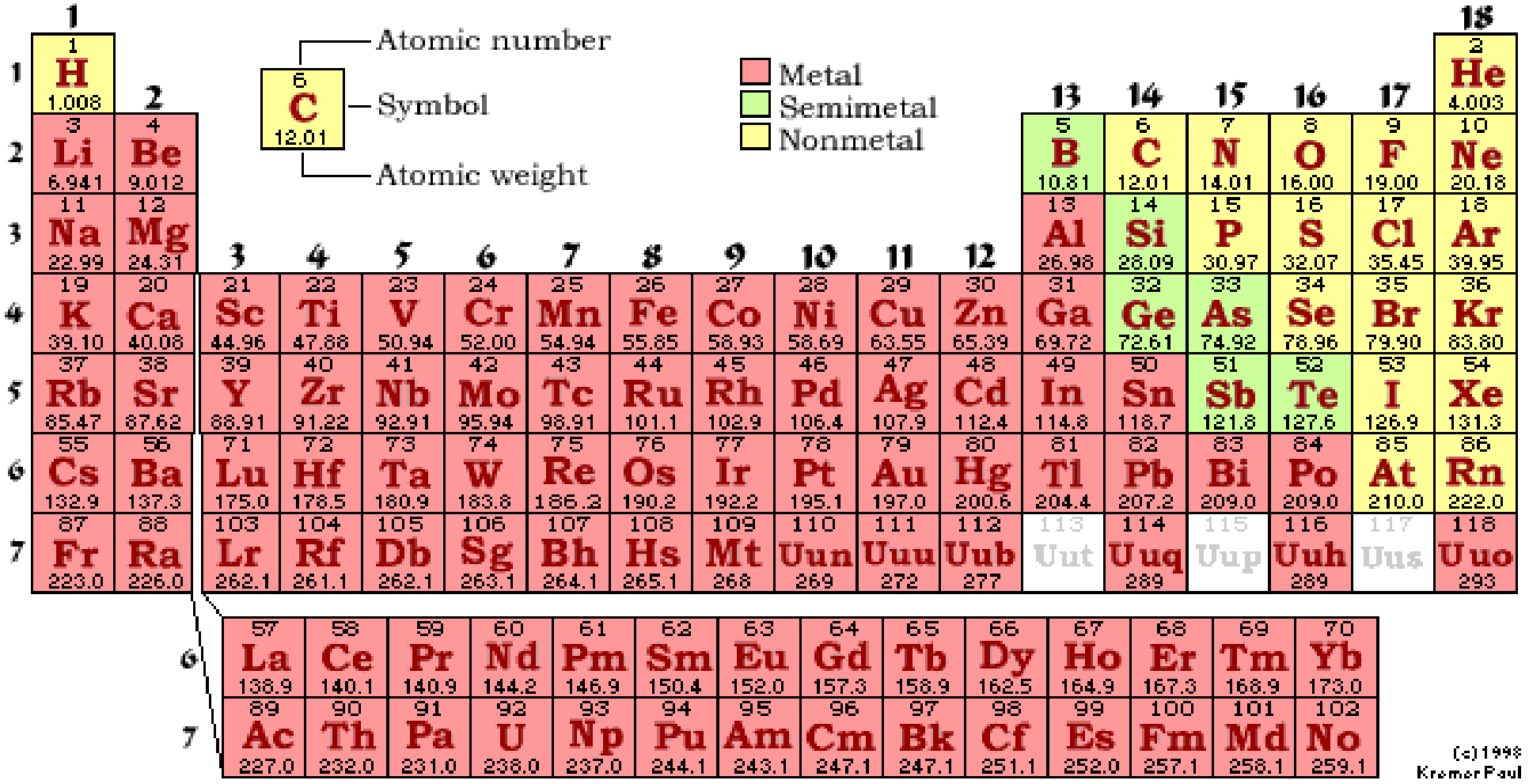
(iv) The onset of the superconducting dome on the under-doped, O / AF side depends on how quickly the upper transitions are suppressed. T_c scales well with T_S and / or T_M.

(v) The onset of the region of e-values that supports superconductivity seems to be associated with a change in the Fermi surface / band structure.

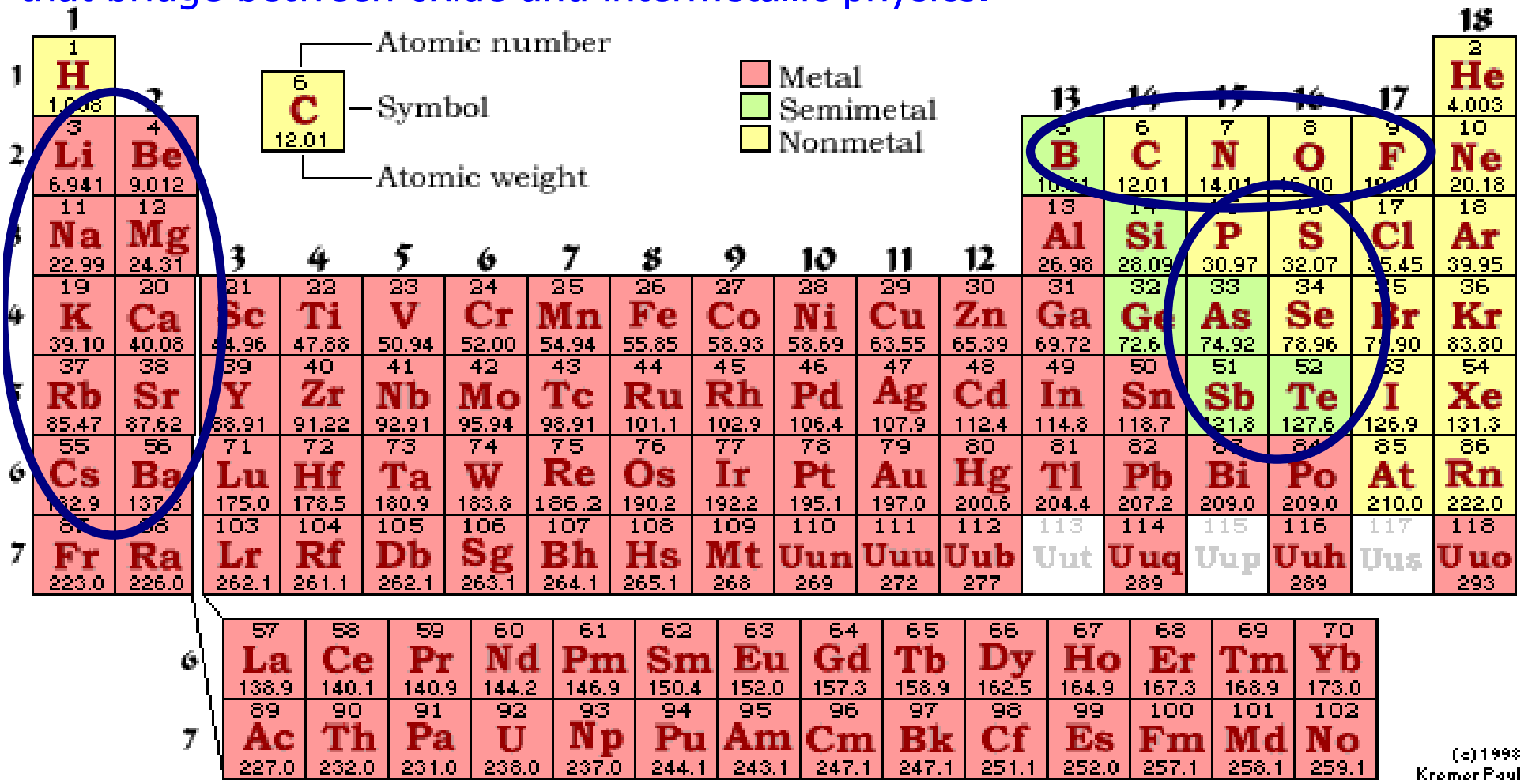
But let's return to looking at the bigger picture,

What can we learn by comparing these examples of "high T_c"?

With H-T_c's, RT_2B_2C, MgB_2, and now FeAs materials we are seeing that compounds that live between traditional oxide physics and intermetallic physics are the ones that offer exciting and potentially useful superconductivity.



With H-T_c's, RT_2B_2C, MgB_2, and now FeAs materials we are seeing that compounds that live between traditional oxide physics and intermetallic physics are the ones that offer exciting and potentially useful superconductivity. Compounds with these elements have been avoided due to the difficulty in making them. These are precisely the compounds that will show properties that bridge between oxide and intermetallic physics.



OK, so what is the way forward then?

Broadly speaking there are two classes of "high T_c" superconductors:

1. Those with the maximum T_c associated with a well defined line compound, e.g. $LuNi_2B_2C$, YPd_2B_2C, MgB_2.

2. Those with the maximum T_c associated with a heavily doped variants of a low T_c or even non-superconducting parent compound, e.g. many of the copper-oxide superconductors and all (so far) of the FeAs superconductors.

There may or may not be a profound physical difference between these classes, but there is a profound difference in the search algorithms that need to be used to try to find them.

With stoichiometric, line compounds there is a good chance of discovering the superconductivity IFF you cool them down to low enough temperature and perform the "right" measurement. (Right being either resistivity or magnetization.)

Remember the MgB_2 $C_p(T)$ data

θ_D

For MgB_2 ~ 750 K

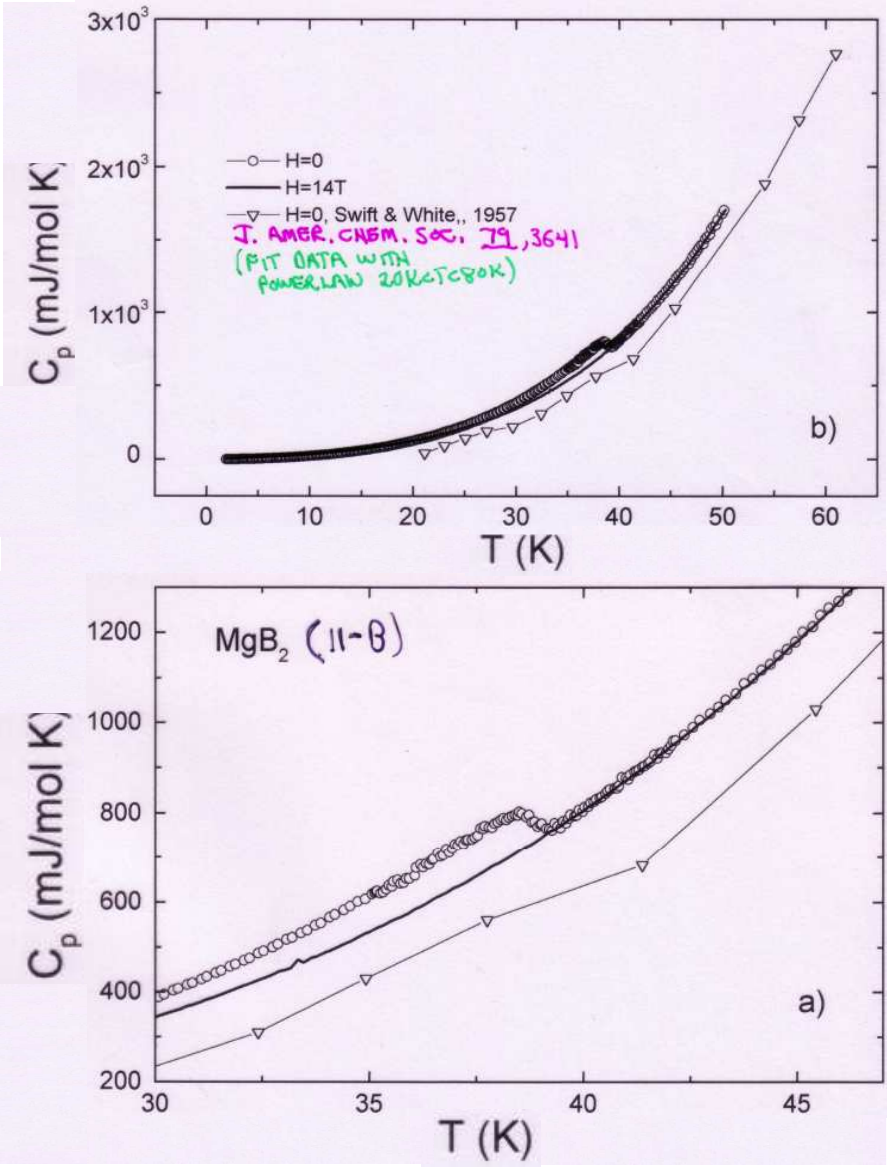
(high ω_D for MgB_2)

$\gamma \sim 2.5 \pm 0.75$ mJ/mole-K^2

(small γ means small $N(E_F)$)

BUT THE TRIANGLELS….

OH, THE TRIANGLES….



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This is a problem of time, numbers and knowledge.

As we have seen so graphically with MgB_2:

(1) not even all the binary compounds have been assessed for superconductivity, let alone ternary, quaternary, etc.

(2) we don't seem to quite know, a priori, where to look…. *(Although post priori we are understanding why more rapidly these days.)*

By developing some basic ideas / sorting mechanisms for limiting phase space searches for new examples of this class of materials have yielded results over the past decades.

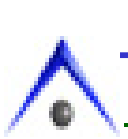
For compounds that manifest the second class of superconductivity, compounds that require "turning on" by *"the right type"* of doping, the discovery of superconductivity is much harder to arrange without some further model or idea of what may be key.

This is a problem of time, numbers, ***numbers again***, and knowledge.

--Very limited types of doping leads to superconductivity in either the copper oxide or FeAs based superconductors.

--Operationally this requires checking several dopings for each host compound to be tested.

--In retrospect we can delineate and perhaps even understand the rules associated with the doping, but a priori this simply means another dimension in an already very large space.



There is a clear and vital need for theoretical / phenomenological support

But sometimes it seems like…

Don't ask what theory can do for you, ask what you can do for theory….(~JFK)

or

…the cops (or theorists) don't need you and man they expect the same….
(~B. Dylan not Queen Jane ~)

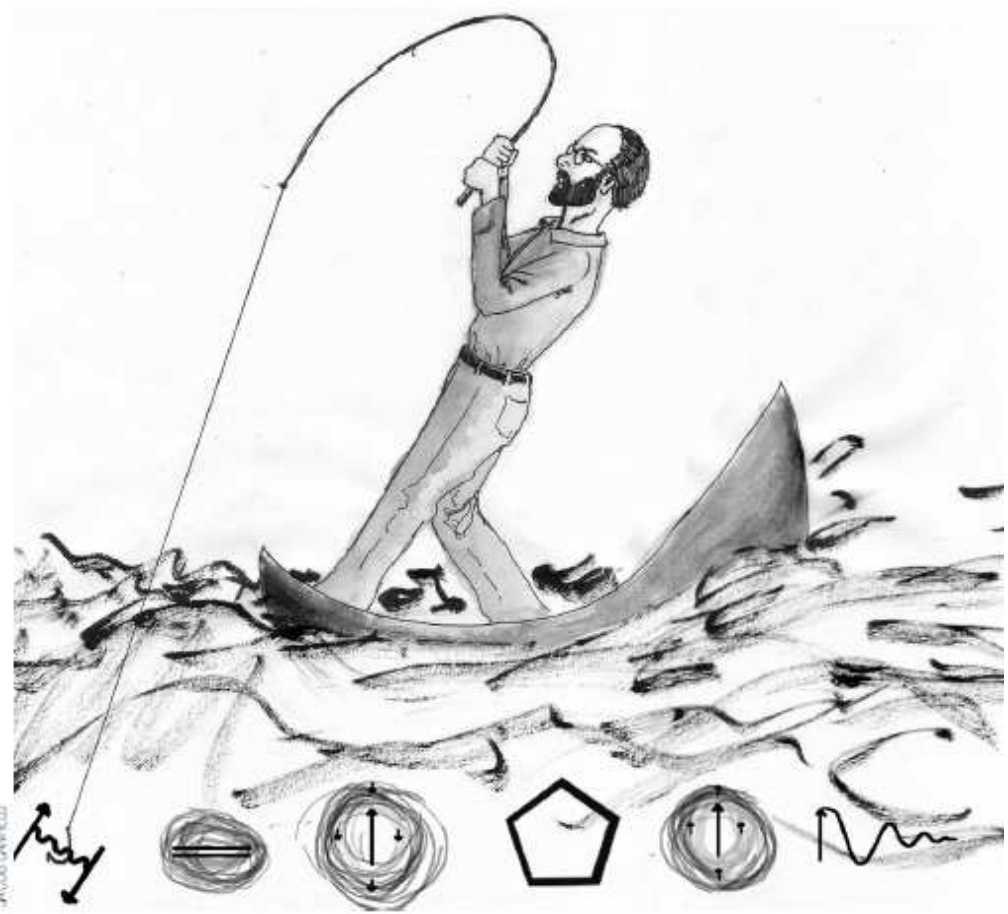
Theory can help by helping to limit phase space

There is a profound need for theory to provide / identify key features or ingredients that can act as sorting parameters to limit the phase space of the search.

What key feature can be generalize from MgB_2 to help us look for other high T_c compounds?

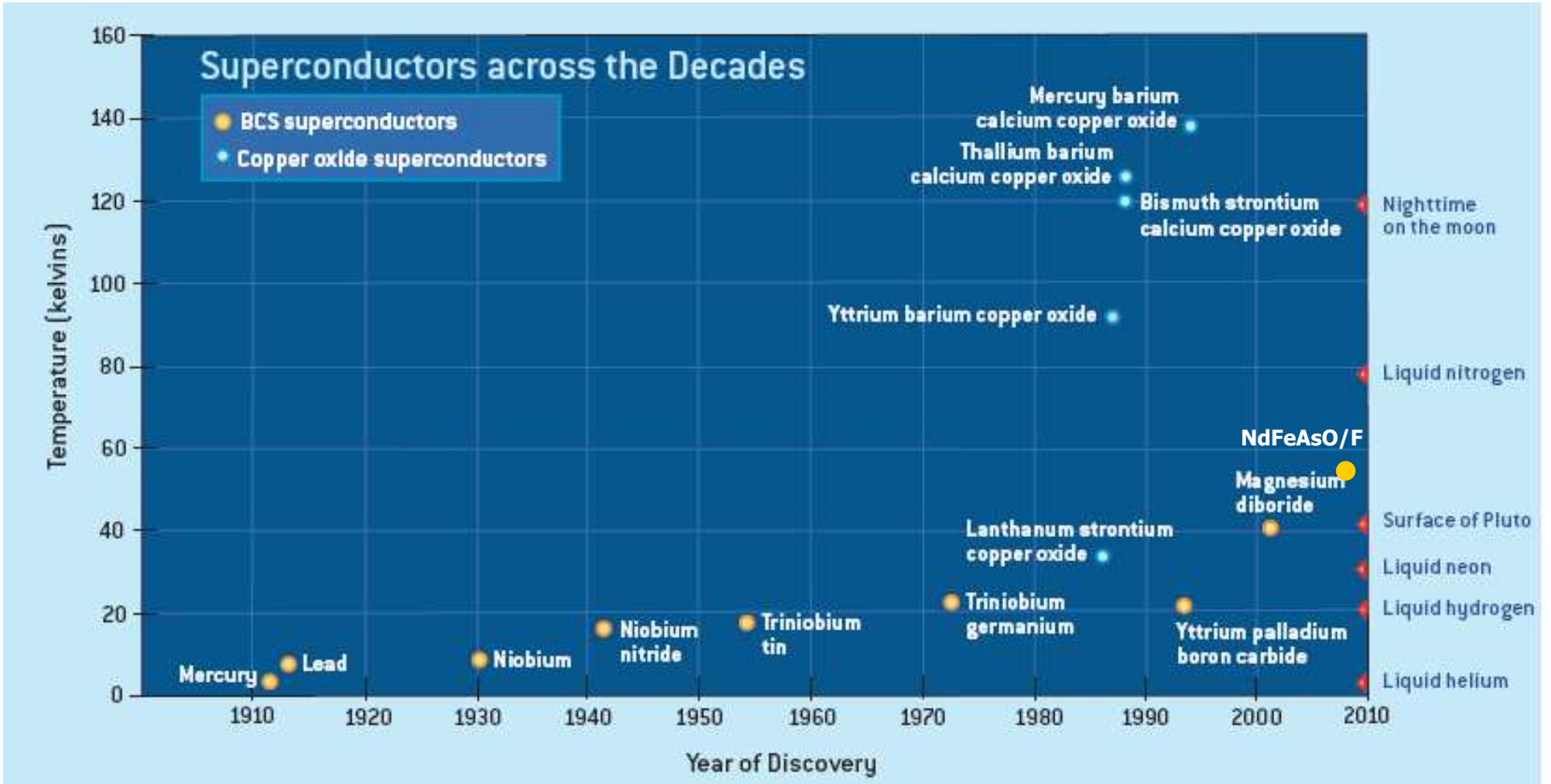
What is special about the FeAs layers in the new superconductors. Can we generalize this to other compounds (away from Fe or away from As)? What phase space is promising, if not that, what phase space is ruled out?

It must be kept in mind (always and humbly) that these are simply rationalizations to search regions of phase space. Although we certainly will find other examples of high T_c superconductivity, the odds are we will discovery it in the compounds we find as a result of a guided walk rather than by purely a priori design.



If possible, it is also important to keep eyes and mind open to the discovery of other interesting systems (CDW, SDW, M-I, etc. transitions or enhanced TEP, normal state diamagnetism, etc.). Just because a compound is not a good superconductor does not mean it is not interesting.

With new searches in poorly explored materials spaces there is promise of exciting discoveries in superconductivity over the next decade. The possibility of an isotropic superconductor with T_c near 100 K (one that would be easy and cheap to make wires from) appears to be getting closer and closer.



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