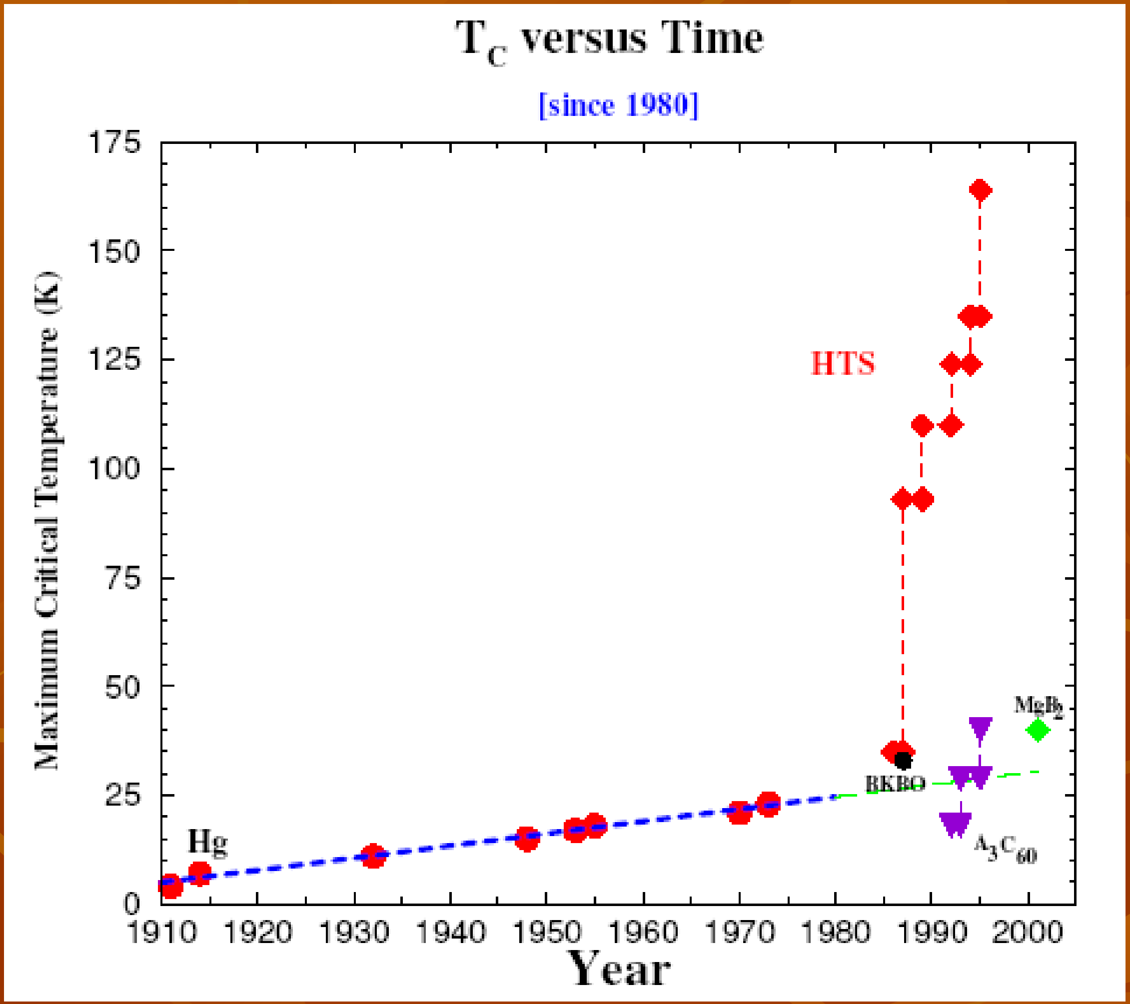
Probing Room Temperature Superconductivity

In A Parallel, Wiser Universe:

Metaphysical Considerations

Warren E. Pickett

Acknowledgment to: Neil Ashcroft


Tc versus Time
[since 1980]
175
150
125
100
75
50
25
0
Maximum Critical Temperature (K)
HTS
MgB2
BKBO
A3C60
Hg
1910 1920 1930 1940 1950 1960 1970 1980 1990 2000
Year

“Matthias’s Rules” for High T_c

- 1. Must have d electrons (not just s-p, nor f)
- 2. High symmetry is good, cubic is best
- 3. Certain electron concentrations are favored
- (peak in density of states at Fermi level)

McMillan (1968)

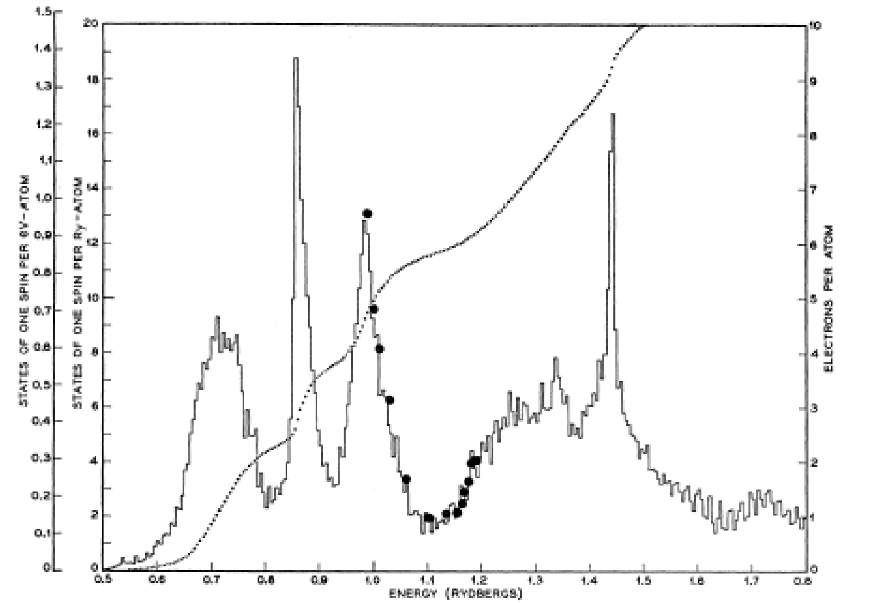
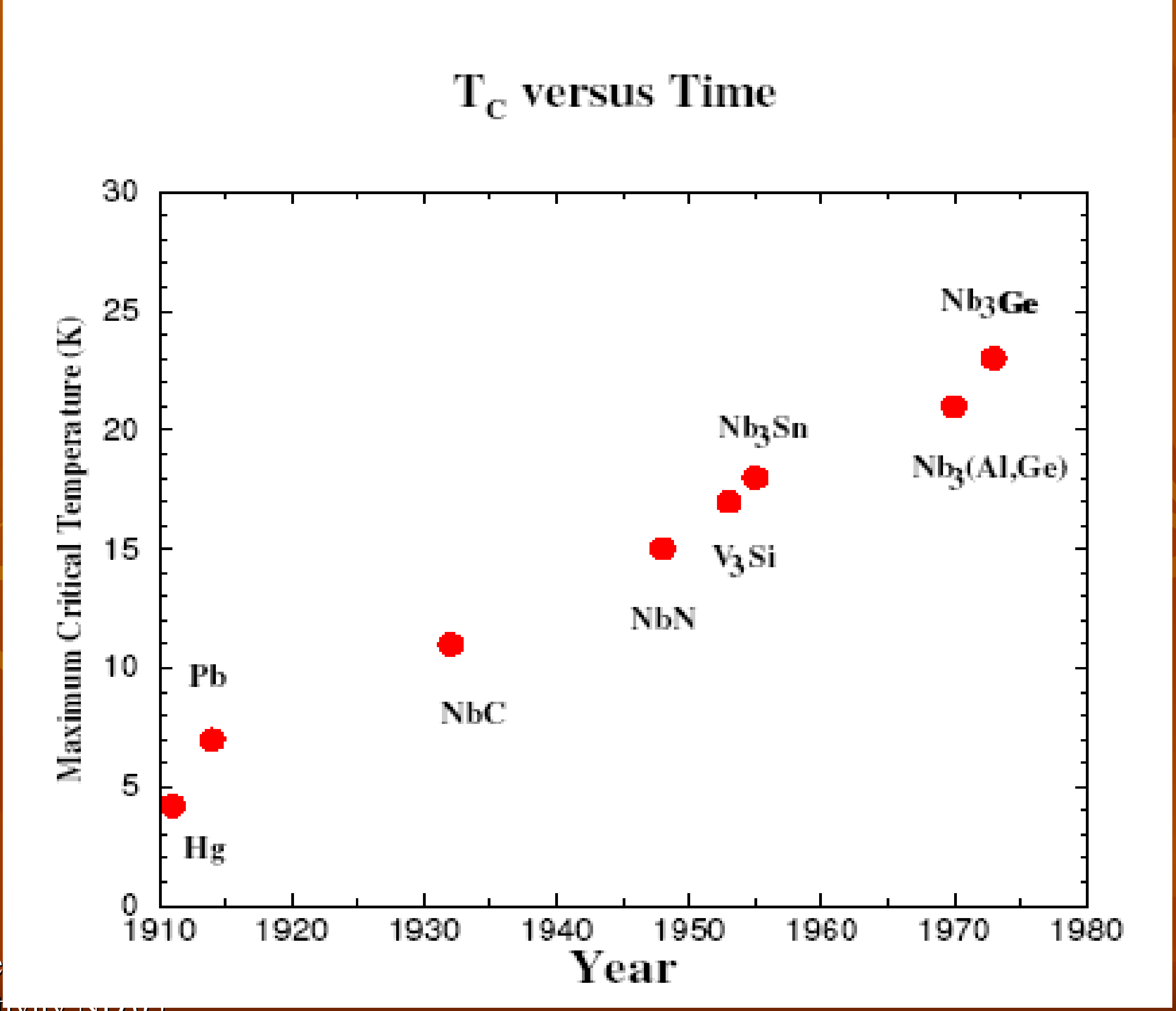
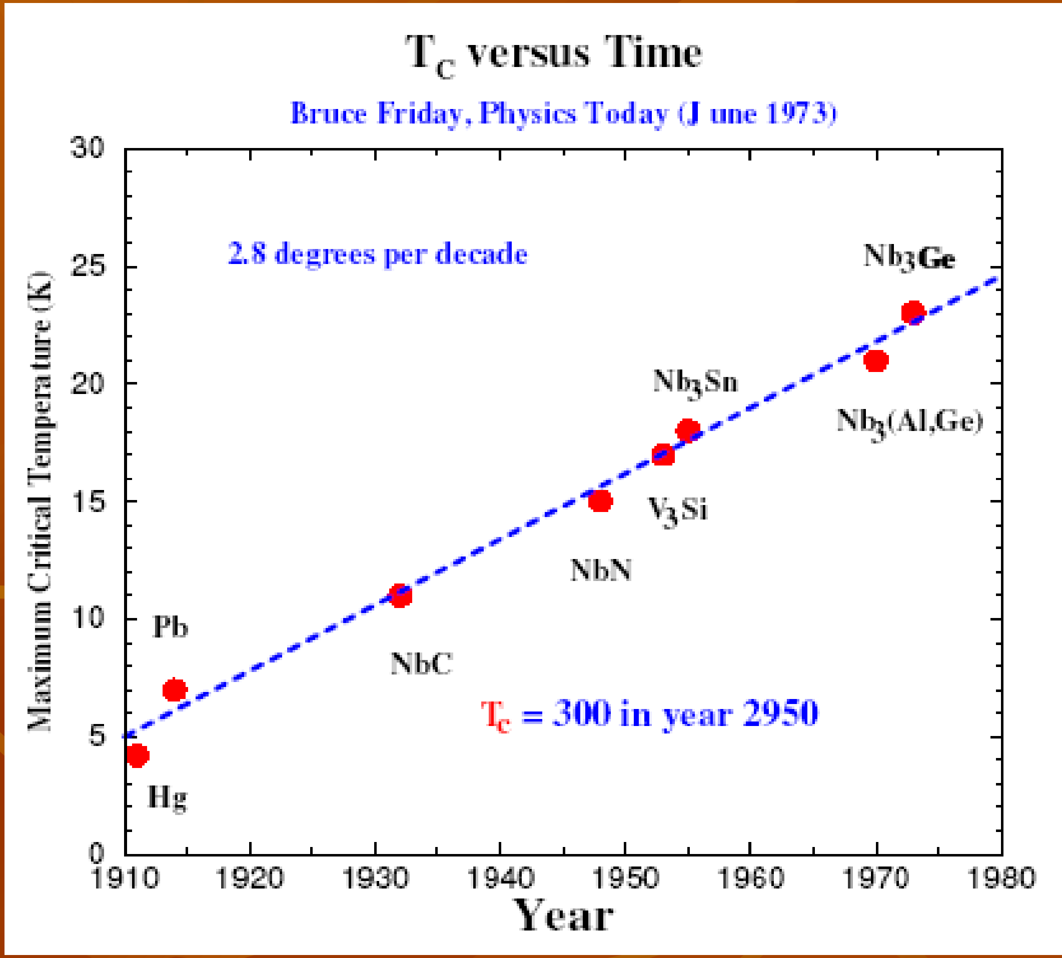


Fig. 10. The theoretical band-structure density of states versus energy for tungsten according to Matthies (Ref. 25), together with the empirical (solid-circles) data for the bcc 5*d* alloys from Tables III and VI.

Advances in the Critical Temperature



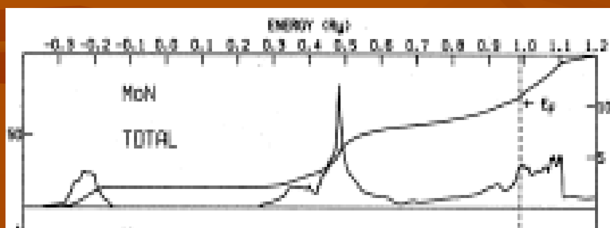
Bruce Friday: Look on the Bright Side

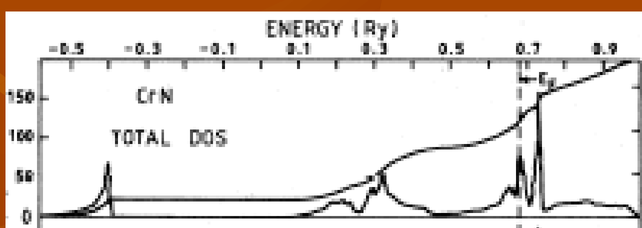


“Nitride Offers 30 K Transition?”

Papaconstantopoulos, WEP, Klein, Boyer, Nature 308, 494 (1984)

MoN: much stronger coupled than Nb(C,N) [T_c = 17 K]





Groups managed to achieve T_c=17 K in MoN_{1-x}, x = 0.9

“Elastic constants of NbC and MoN: instability of B1-structure MoN.”
Chen, Boyer, Krakauer, Mehl, PR B (1988)

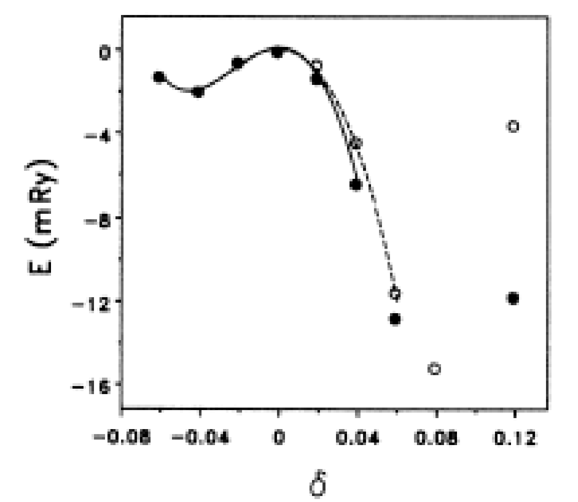
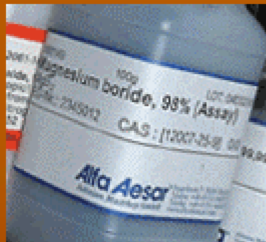


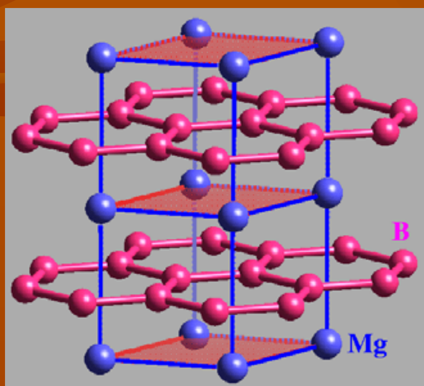
FIG. 3. The solid circles are calculated total energies for small trigonal distortions of B_1-MoN, while the open circles are for its orthorhombic distortions. The values are given relative to the energy of the B_1 structure which is −8199.462 25 Ry, and the relative energies for the orthorhombic distortions have been multiplied by 3. The lines are the least-squares fit in small regions around the B_1 structure.



Akimitsu's Discovery: 2001

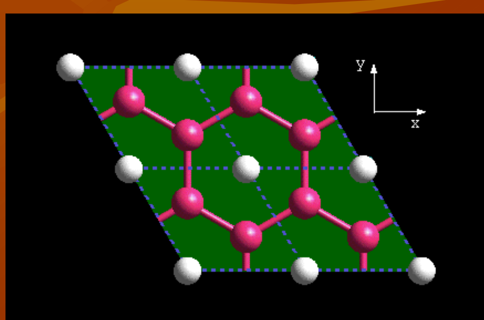
MgB_2, a common chemical reagent.

Searching for ferromagnetism, superconductivity at 40 K was discovered



Quickly reproduced and synthesis techniques were extended by several groups

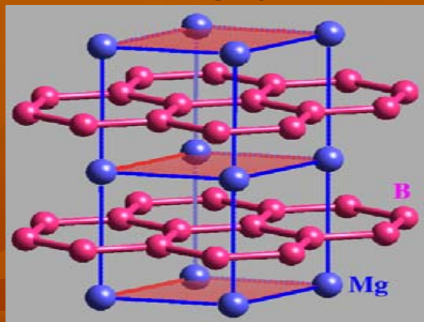
Crystal structure is simple. Quasi-2D.

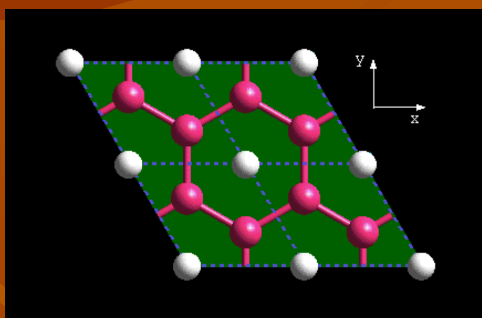


Electronic structure is simple: s-p electrons.

Nagamatsu, Nakagawa, Muranaka, Zenitani, and Akimitsu, Nature **410**, 63 (2001)

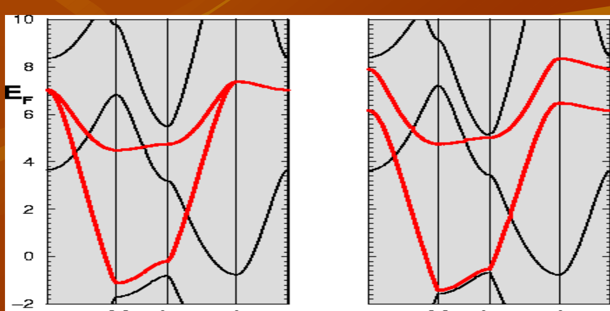
Four Months Later: Puzzle Solved!



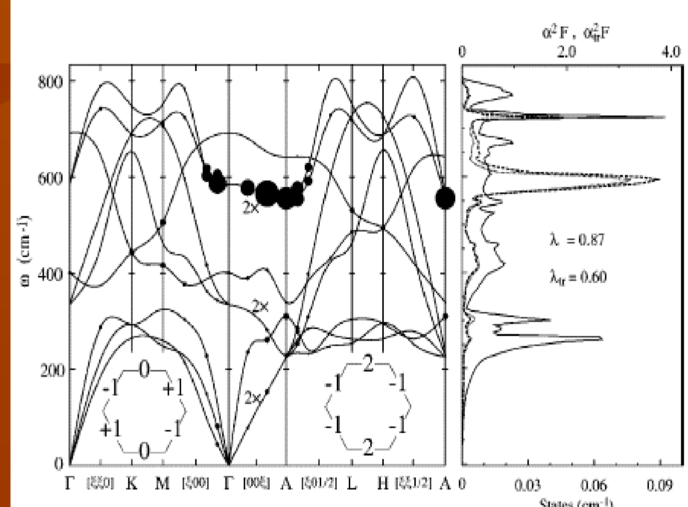


1. MgB_2: covalent bonds become metallic
2. Deformation potential *D*=13 eV/A
   (amazingly large for a metal)
3. 2D (cylinder) Fermi surfaces focus strength
4. Yet structure remains stable: intrinsic covalency

J. M. An and WEP, Phys. Rev. Lett. (2001)
J. Kortus et al., Phys. Rev. Lett. (2001)
Y. Kong et al., Phys. Rev. B (2001)
K.-P. Bohnen et al., Phys. Rev. Lett. (2001)
……..more…….



T. Yildirim (NIST)



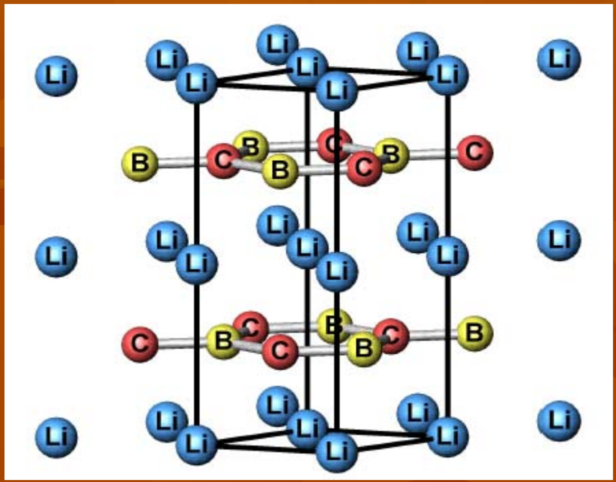
Y. KONG, O. V. DOLGOV, O. JEPSEN, AND O. K. ANDERSEN

PHYSICAL REVIEW B 64 020501(R)

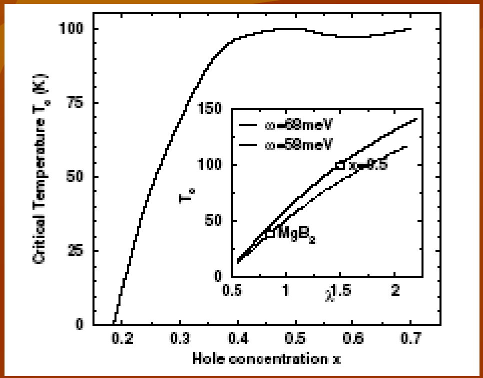
FIG. 1. Left: Calculated phonon dispersion curves in MgB_2. The area of each circle is proportional to the mode λ. The insets at the bottom show the two ΓA E eigenvectors (not normalized), which apply to the holes at the top of the σ bands (bond-orbital coefficients) as well as to the optical bond-stretching phonons (relative change of bond lengths). Right: $F(\omega)$ (full curve and bottom scale), $\alpha^2(\omega)F(\omega)$ (broken), and $\alpha^2_{tr}(\omega)F(\omega)$ (dotted). See text.

Prediction of a "better MgB_2": $Li_{1-x}BC$

Rosner, Kitiagorodsky, WEP, Phys. Rev. Lett. (2002)



Structurally, chemically, similar to MgB_2
Semiconductor, so hole-doping is required
(de-intercalation of Li)
Deformation potential 50% larger than MgB_2
T_c =75 K might be realistic estimate



Not so simple!

Several reports of inability to prepare $Li_{1-x}BC$

Reports that $Li_{1-x}BC$ is not superconducting:

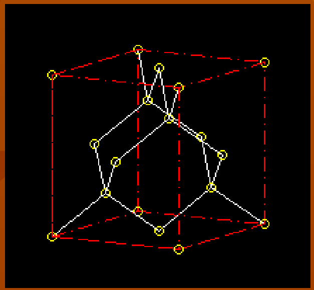
Zhao, Klavins, Liu, J. Appl. Phys. (2003)
Fogg, Claridge, Darling, Rosseinsky (2003)

But the $Li_{1-x}BC$ samples are not well characterized.

physicsweb Physics news, jobs and resources

$T_c = 8$ K

- **Superconducting diamond turns up in Russia**
- 31 March 2004
- **Physicists at the Russian Academy of Sciences are claiming to have created a form of diamond that superconducts. Vladimir Sidorov and colleagues say that their material, which they made by doping carbon with boron at high temperatures and pressures, exhibits bulk superconductivity below around 4 kelvin and remains a superconductor in strong magnetic fields (E A Ekimov *et al.* 2004 *Nature* 428 542).This is the first time that boron-doped diamond -- which is normally a semiconductor -- has shown superconducting behaviour.**



Boeri, Kortus and Andersen, PRL 93, 237002 (2004)
K.-W. Lee and WEP, PRL 93, 237003 (2004)
Xiang, Li, Yang, Hou, Zhu, PR B 70,212504 (2004)
Blasé, Adesssi, Connetabable, PRL 93, 237004 (2004)
G. Baskaran, cond-mat/0404286.

Heavy vs. Light Elements

"McMillan's equation"

$$T_c = \frac{\langle \omega \rangle}{1.20} \exp\left(- \frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right)$$

Ashcroft (1962----)

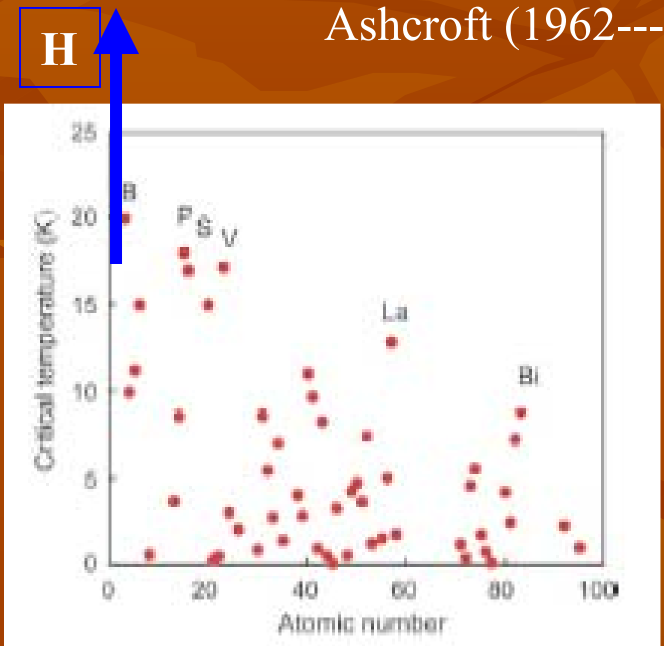


Figure 11. Highest critical temperature of simple elements as a function of the atomic number.

Cristina Buzea [1,2] * and Kevin Robbie [1,2]

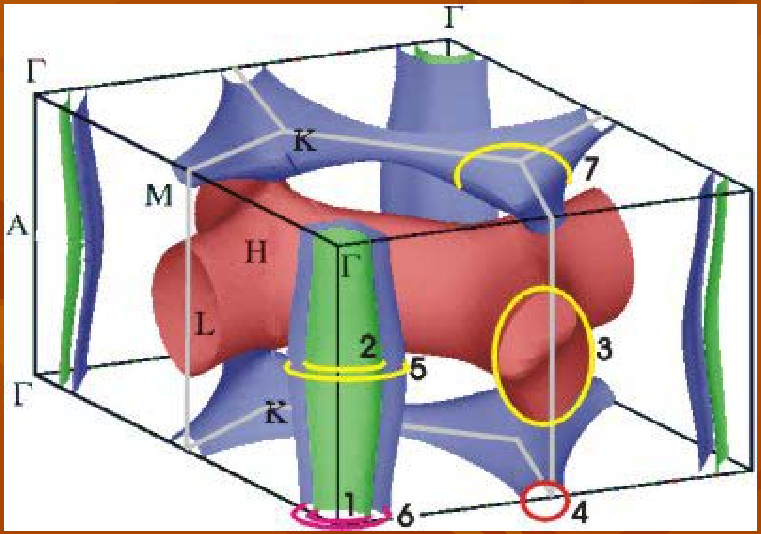
to appear in Supercond. Sci. Technol. 18 (2005) R1-R8

Lighter elements can be favorable for raising the critical temperature

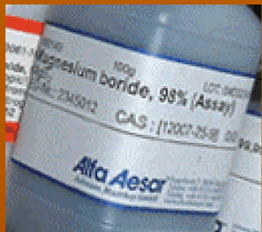
MgB_2: light metal atom, lighter metalloid

2001-2003: a Paradigm Shift

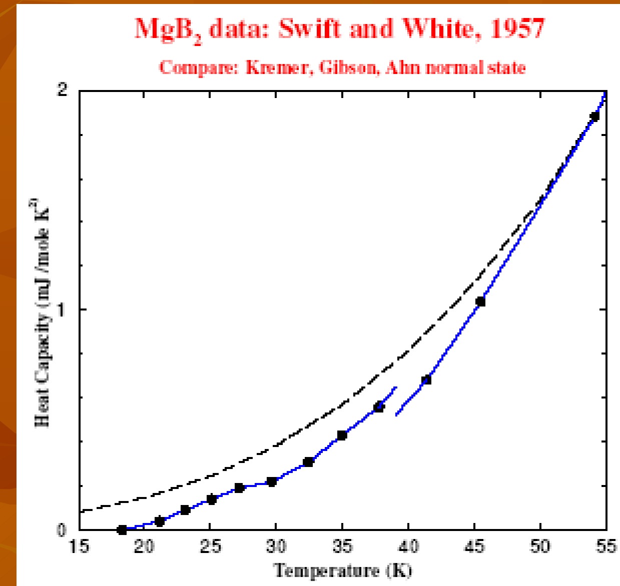
- What is possible regarding strong coupling in el-ph coupled s-p electron superconductors
- Two-gap superconductivity: a new form of extreme anisotropy

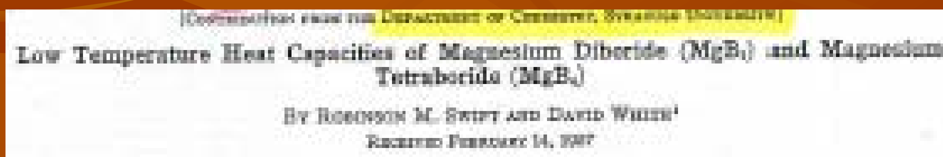


....in this universe....



MgB_2 in 1957





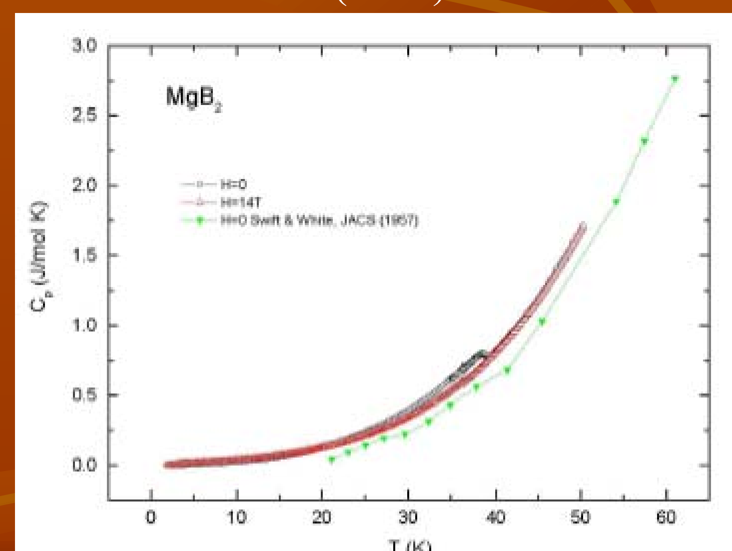
[Contribution from the Department of Chemistry, Syracuse University]

Low Temperature Heat Capacities of Magnesium Diboride (MgB_2) and Magnesium Tetraboride (MgB_4)

By Robinson M. Swift and David White[1]

Received February 14, 1957

Canfield (2003)



- In another universe, developments paralleled those in our universe up to 1957. In that universe, however, Robinson Swift and David White recognized the superconductivity in MgB_2, and the two universes went their separate ways………

Through means to be described elsewhere,[1] some of the subsequent developments in this universe have been uncovered….

[1] N. W. Ashcroft and W. E. Pickett, another time, another universe.

Our Universe

1955 T_c=18 K in Nb_3Sn

1957 BCS theory

1958 Matthias's rules: d electrons; high DOS, symmetry is good, cubic is best

1960 A15 research ramps up (no increase in T_c is found)

1962 N. Ashcroft predicts Tc>100 K in metallic hydrogen

1963 A15 research intensifies……….

That Universe

1955 T_c=18 K in Nb_3Sn

1957 BCS theory

Swift & White: T_c=40 K in MgB2

1958 Swift&White rules: s-p electrons are best; DOS is not important; layers are fine

1960 Emphasis moves to light atoms; A15 research is cut dramatically

1962 N. Ashcroft predicts T_c>100 K in metallic hydrogen

1963 Intercalated graphite (structural similarity to MgB_2) studied, T_c up to 5 K

Our Universe

1964 W. Little presents case for excitonic sc'y in organic polymers

1966 Structural instabilities in A15s attract much interest and study

1968 Tunneling studies of A15 compounds are hampered by materials difficulties

1970 T_c=21 K in Nb_3(Al,Ge). Wow!

1972 BCS win Nobel Prize (Physics)

That Universe

1964 Polymeric $(BeH)_x$ synthesized, black and flubberlike; has T_c=55 K but transforms to an insulator at 40 K

1966 LiBC, isostructural and isoelectronic to MgB_2, is synthesized

1968 LiBC is hole-doped electrochemically, T_c = 94 K is achieved

1970 Hexaboride $(H_2)_xB_6$, 5<x<7, is synthesized; T_c=70 K

1972 BCS win Nobel Prize (Physics)

S&W win Nobel Prize (Chemistry)

Our Universe

1974 Tc=23.1 K achieved in Nb_3Ge
Disallusionment with A15s settles in
B. Friday tries to encourage with $T_c(t)$

1975 Allen-Dynes theory: there's not really any limit to T_c, except stability

1978 Theorists argue that structural instabilities limit T_c to less than 30 K

1986 Ferroelectricity experts Bednorz and Mueller find T_c=30 K in $(La,Ba)_2CuO_4$

1987 APS March Meeting "Woodstock Session" lasts until 5 AM.

Now T_c = 93 K in $YBa_2Cu_3O_7$ (Chu)

That Universe

1975 Mao and Bell achieve Mbar pressure in Li, find T_c=20 K

1978 T_c=98 K in $Li_2H_3BeB_4$
(light atoms, covalent bonding)

1982 Metastable $LiBeN_3$ (perovskite) becomes ferroelectric at 540 K, then transforms to sc'ing at 235 K. Current flow charges the samples, then kills sc'y. Current relaxes, FE state returns, then sc'y…. Over and over, at rate of 38 GHz → 3K (temperature units). Interstellar $LiBeN_3$ becomes the prime candidate for the cosmic 3 degree background.

1986 Ferroelectricity experts Bednorz and Mueller find T_c=30 K in $(La,Ba)CuO_4$. Reproducible, but samples are messy and uninteresting, and are discarded

# Our Universe	# That Universe
2001 Akimitsu discovers T_c=40 K in MgB_2. APS "Woodstock II" lasts until 2 AM.	1996 Superconducting SuperCollider completed on schedule, thanks partly to \$600M saving from HTS (Li_xBC) technology at LN_2 temperature (77 K)
2003-4 Three groups find T_c=18-20 K in Li around 400 kbar	2005 Janko and collaborators announce an entirely new compound that superconducts at 302 K, it is…….

patent pending

Insight from a Great Metaphysicist

"There is no question there is an unseen universe.
The question is: how far is it from midtown, and how late it is open?"

Woody Allen

Summation

MgB_2 introduced a new paradigm in strong-coupling superconductors

[45 years later than it should have]

[A_3C_{60} (A = alkaline metal K, Rb, Cs), T_c up to 40 K, represents another new paradigm (vaguely related, but clearly different)]

Great leaps in superconductivity seem to require new paradigms

What we 'know' is limited by what we have not yet discovered

What we are, and what we do now, is determined by when we discover it as well as what we discover