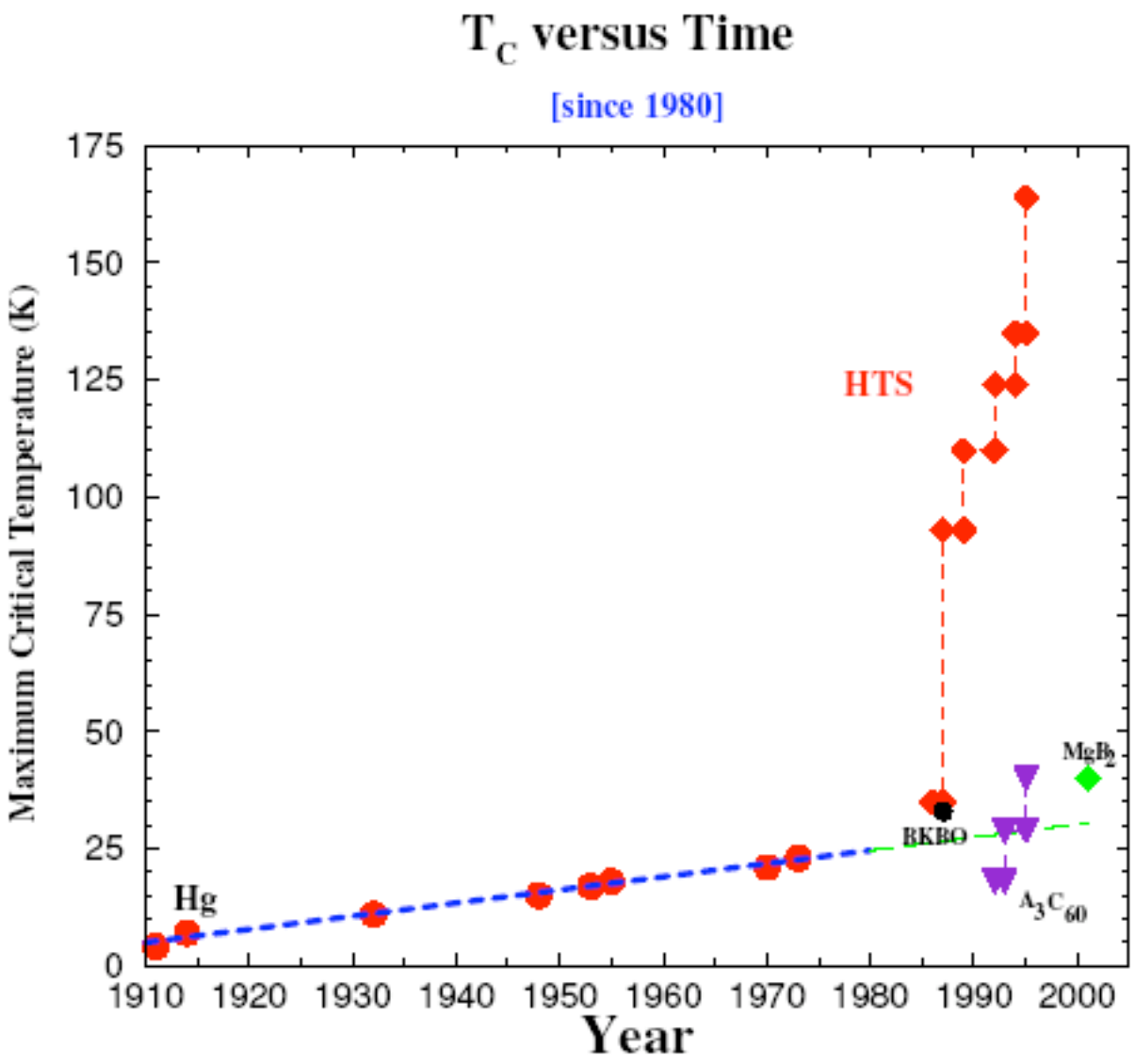
Electron-Phonon Coupling: when Conventional becomes Unconventional

Warren E. Pickett, UC Davis

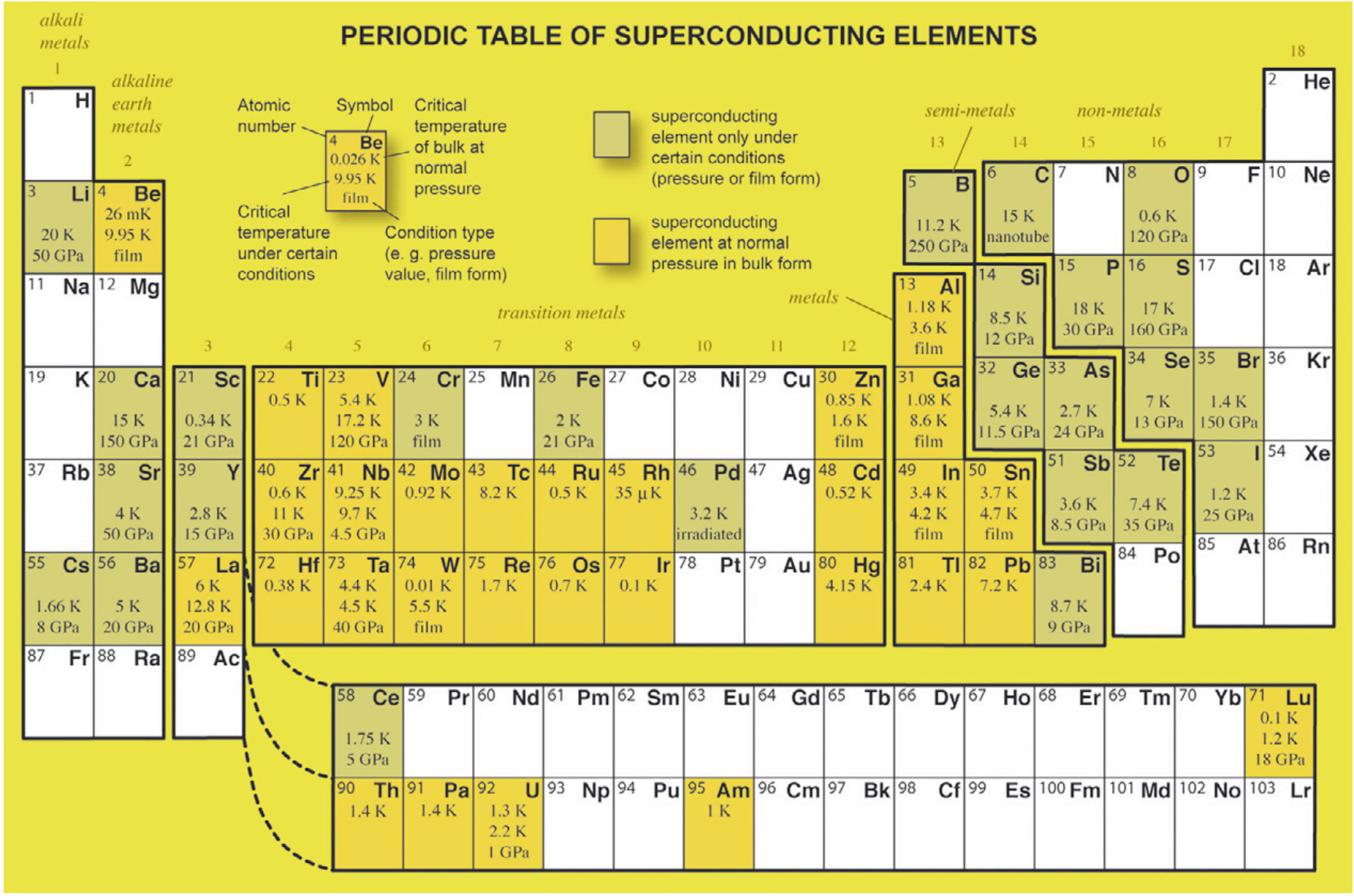
Acknowledgments: within the talk

Summer School on Novel Superconductivity, August 2009


T_C versus Time
[since 1980]
Maximum Critical Temperature (K)
175
150
125
100
75
50
25
0
1910
1920
1930
1940
1950
1960
1970
1980
1990
2000
Year
HTS
Hg
BKBO
MgB_2
A_3C_{60}

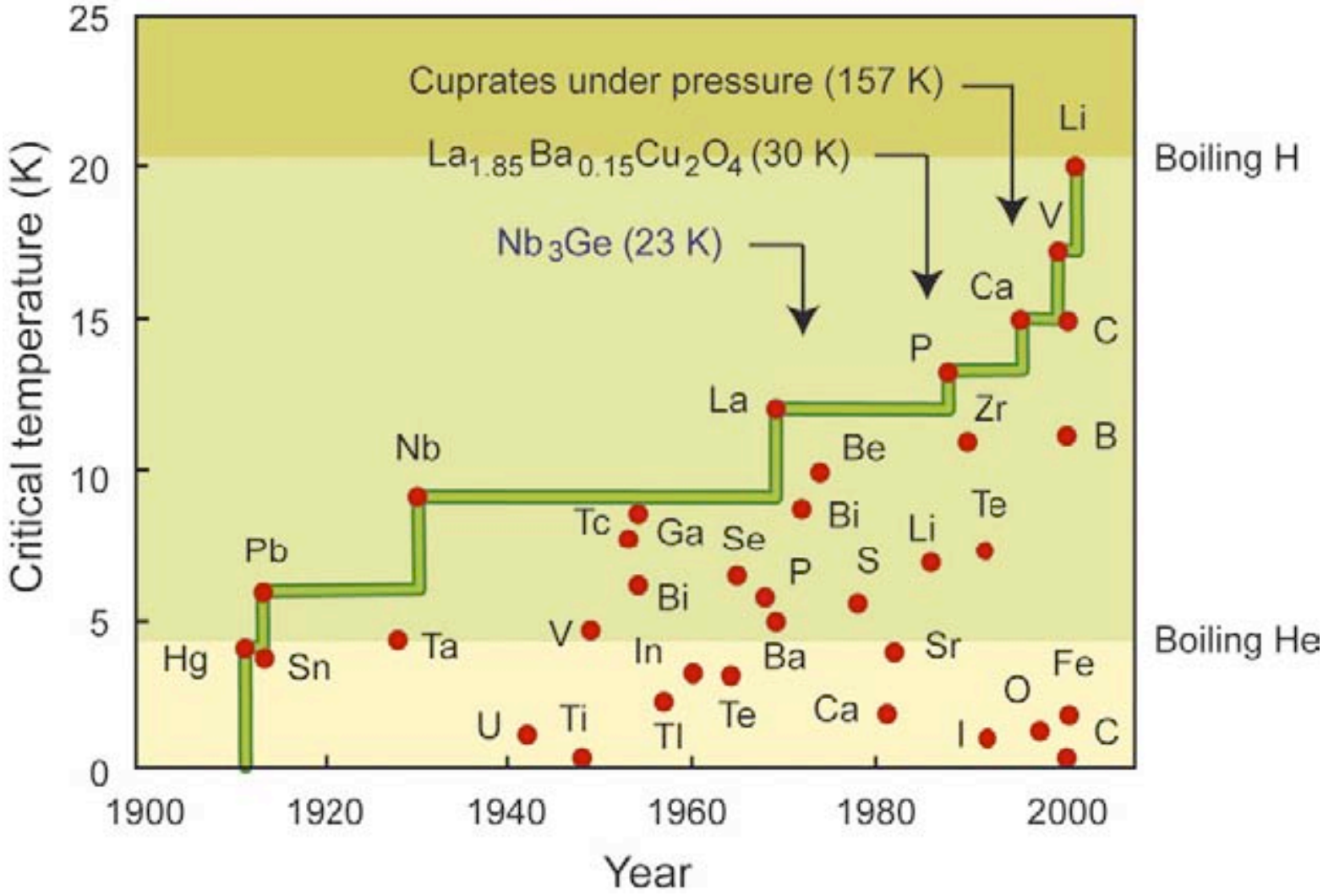
The Other High Temperature Superconductors

56 K Fe-pnictides: class of doped ROFeAs (R = rare earth ion)
40 K MgB_2: a new s-p class with only one member (?$C_{2-x}B_x$?)
40 K Cs_3C_{60}: the lowest density A_3C_{60} fulleride
35 K (Ba,K)BiO_3 (BKBO): s-p system, no excuse for this Tc
25 K $Li_x(ZrNCl)_2$: 2D layers, simple(?), low N(0)
20 K Li at 40 GPa: simple 2s metal pushed to its limits (2p)
19 K $PuCoGa_5$: 5f electron system, a new game entirely

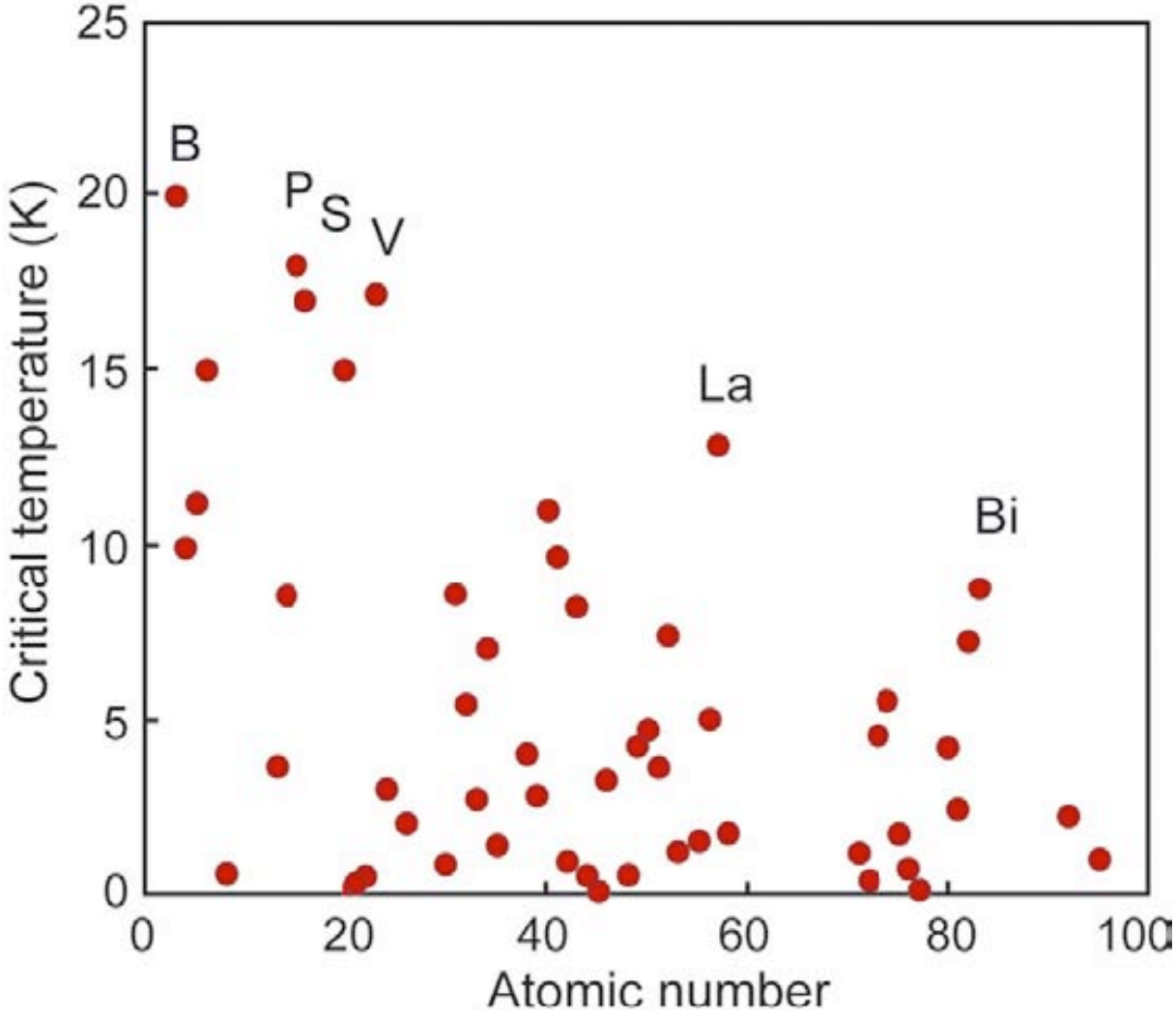


Y 20 K at 115 GPa, Ca 25 K at 161 GPa

C. Buzea *et al.,* Supercond. Sci. Technol. **18** (2005) R1–R8



Historical development of the critical temperature of simple elements
(C. Buzea *et al.,* Supercond. Sci. Technol. **18** (2005) R1–R8)



Highest critical temperature of simple elements as a function of the atomic number.
(C. Buzea *et al.,* Supercond. Sci. Technol. **18** (2005) R1–R8)

Electron-Phonon Coupling

Hamiltonian for band electrons coupled to harmonic phonons:

$$
\begin{aligned}
H_{e-ph} &= \sum_{ks} \epsilon_{ks} c^{\dagger}_{ks} c_{ks} \\
&+ \sum_{q\nu} \hbar\omega_{q\nu} (b^{\dagger}_{q\nu} b_{q\nu} + \frac{1}{2}) \\
&+ \sum_{ks} \sum_{q\nu} [M^{\nu}_{k,q} c^{\dagger}_{k+q,s} c_{k,s} b_{q\nu} + h.c.]
\end{aligned}
$$

The electron phonon matrix element

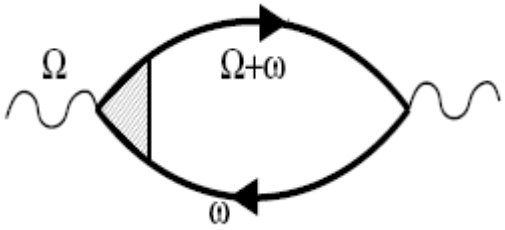
- The definition is the probability of scattering from the one-electron state $|\boldsymbol{k}j\rangle$ to the state

  $|\boldsymbol{k}+\mathbf{Q}\ j'\rangle$ via the phonon $\mathbf{Q}v$
- Mathematically:

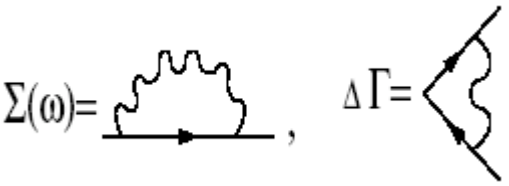
$$M^{\vec{Q}v}_{\vec{k}+\vec{Q}j',\vec{k}j} = \left\langle \vec{k}+\vec{Q}j' \middle| \delta^{\vec{Q}v} V_{eff} \middle| \vec{k}j \right\rangle$$

Phonon-paired Superconductivity

Electrons become paired by (attractive) exchange of virtual phonons, which overcomes the (repulsive) electron-electron repulsion if the el-ph coupling is sufficiently strong. Pairs coalesce into a macroscopic broken-gauge-symmetry state with long-range phase coherence.



Phonon self-energy bubble: electron-hole pair creation and reabsorption



Electron self-energy: phonon emission and reabsorption

"Migdal's theorem": vertex corrections are order m/M (negligible) in normal state

Electron-Phonon Coupling: General Results for $\lambda_{Q\nu}$ and $\gamma_{Q\nu}$

P. B. Allen, PR B6, 2577 (1972)

$$
\begin{aligned}
\lambda &= \frac{1}{N_\nu}\sum_{Q,\nu=1}^{N_\nu}\lambda_{\vec{Q},\nu} = 2\int\frac{\alpha^2F(\omega)}{\omega}d\omega \\
\alpha^2F(\omega) &= \frac{2}{\pi N(0)\omega}\sum_{Q\nu}\gamma_{Q\nu}\delta(\omega_{Q\nu}-\omega) \\
\omega_{Q\nu}^2 &= \Omega_{Q\nu}^2 + 2\Omega_{Q\nu}^2 Re\ \Pi(Q,\omega_{Q\nu}) \\
\gamma_{Q\nu} &= \frac{\Omega_{q\nu}}{\omega_{Q\nu}} Im\ \Pi(Q,\omega_{Q\nu}) \\
&= \pi\sum_k |M_{k,k+Q}|^2\delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) \\
\lambda &= \frac{1}{N_\nu}\sum_{Q\nu}\lambda_{Q\nu} = \frac{4}{\pi N(0)}\sum_{Q\nu}\frac{\gamma_{Q\nu}}{\omega_{Q\nu}^2}
\end{aligned}
$$

Formalism: Electron-Phonon Coupling

Phonon scattering electron: from Fermi surface to Fermi surface

The electron-phonon coupling strength for phonon $(\vec{Q}, \nu)$ is given by[1]

$$\lambda_{\vec{Q},\nu} = 4\frac{2}{\omega_{\vec{Q},\nu}} \sum_k |M_{k,k+Q}|^2 \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = 4\frac{2V_c}{\omega_{\vec{Q},\nu}} |M|^2 \int_{\mathcal{L}} \frac{d\mathcal{L}(k,Q)}{|\vec{v}_k \times \vec{v}_{k+Q}|} \qquad (1)$$

$$\xi_{\vec{Q}} = \sum_k \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = V_c \int_{\mathcal{L}} \frac{d\mathcal{L}(k,Q)}{|\vec{v}_k \times \vec{v}_{k+Q}|}$$

$\mathcal{L}$ is the line of intersection between the Fermi surface, and its $\vec{q}$-displaced image.

Phonon softening: electron-hole pair emission/reabsorption

The phonon frequency is renormalized downward by the strong coupling, which is expressed in terms of the associated phonon self-energy $\Pi(Q,\omega)$:

$$\omega_{Q\nu}^2 = \Omega_{Q\nu}^2 + 2\Omega_{Q\nu}^2 \Pi(Q, \omega_{Q\nu})$$

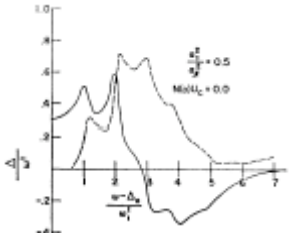
$$\Pi(Q,\omega) = -2 \sum_k |M_{k,k+Q}|^2 \frac{f_k - f_{k+Q}}{\varepsilon_{k+Q} - \varepsilon_k - \omega - i\delta},$$

Theory of Strong Coupling Superconductivity

G. M. Eliashberg, Sov. Phys. JETP (1960)
Scalapino, Schrieffer, Wilkins, Phys. Rev. (1966)

Starting from full electron+nuclei Hamiltonian

* Presume electrons form a Fermi liquid state
* Presume stable structure→conventional phonons
* Presume conventional el-ph theory holds (Migdal's theorem)
* Presume el-el interaction is not anomalous



Complex-valued energy-dependent gap function for Pb

Rowell, McMillan, Feldman (1969)

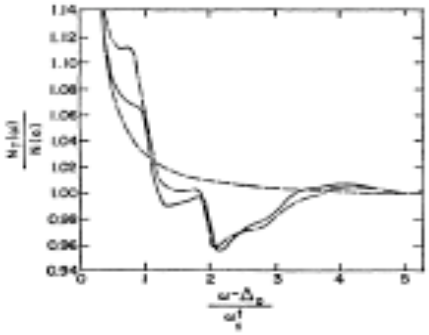


FIG. 10. The effective tunneling density of states $N_T(\omega)/N(0) = \mathrm{Re}\{\omega/(\omega^2-\Delta^2(\omega))^{1/2}\}$ versus $(\omega-\Delta_0)/\omega_1'$ (solid) obtained from Δ of Fig. 8. The ratio of the differential conductance of Pb in the superconducting to that in the normal state (Ref. 25) is plotted (dash-dot) as a function of $(\omega-\Delta_0)/\omega_1'$. The prediction of the simplified BCS model $\omega/(\omega^2-\Delta_0^2)^{1/2}$ is shown as the short dashed curve.

Electron-Phonon Coupling:
General Results for $\lambda_{Q\nu}$ and $\gamma_{Q\nu}$
P. B. Allen, PR B6, 2577 (1972)

$$\lambda = \frac{1}{N_\nu}\sum_{Q,\nu=1}^{N_\nu}\lambda_{Q,\nu} = 2\int\frac{\alpha^2F(\omega)}{\omega}d\omega$$

$$\alpha^2F(\omega) = \frac{2}{\pi N(0)\omega}\sum_{Q\nu}\gamma_{Q\nu}\delta(\omega_{Q\nu}-\omega)$$

$$\omega_{Q\nu}^2 = \Omega_{Q\nu}^2 + 2\Omega_{Q\nu}^2 Re\ \Pi(Q,\omega_{Q\nu})$$

$$\gamma_{Q\nu} = \frac{\Omega_{q\nu}}{\omega_{Q\nu}} Im\ \Pi(Q,\omega_{Q\nu})$$

$$= \pi\sum_k |M_{k,k+Q}|^2\delta(\varepsilon_k)\delta(\varepsilon_{k+Q})$$

$$\lambda = \frac{1}{N_\nu}\sum_{Q\nu}\lambda_{Q\nu} = \frac{4}{\pi N(0)}\sum_{Q\nu}\frac{\gamma_{Q\nu}}{\omega_{Q\nu}^2}$$

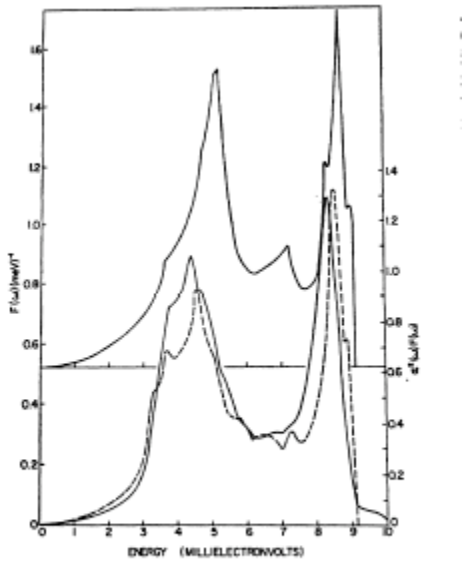


FIG. 1. Upper trace shows the phonon density $F(\omega)$ in Pb taken from Ref. 1. The lower dashed curve is the phonon density from Ref. 8. The area under the spectrum is normalized to 3. The lower solid line is the function $\alpha^2(\omega)F(\omega)$ determined from superconducting tunneling.

TABLE II. Values of λ for superconducting crystalline elements

Metal	T_c(K)	Θ_D(K)	λ_{McM}[a]	λ_{tr}	λ_{tun}	λ_{LDA}
Be	0.026	1390	0.23			
Al	1.16	428	0.38	0.39[b]		0.44[c,d]
Zn	0.85	309	0.38	0.46[e]		
α-Ga	1.08	325	0.40			
β-Ga	5.9				0.97[f]	
Cd	0.52	209	0.38	0.37[e]		
In	3.40	112	0.69		0.834[g]	
Sn	3.72	200	0.60		0.72[h]	
Hg	4.16	72	1.00		1.60[i]	
Tl	2.38	79	0.71	1.11[e]	0.78[f]	
Pb	7.19	105	1.12	1.48[b]	1.55[j]	1.20[d],1.68[c]
Ti	0.39	425	0.38	0.50[k]		
V	5.30	399	0.60	1.09[b]	0.83[l]	1.19[c]
Zr	0.55	290	0.41	0.55[k]		
Nb	9.22	277	0.82	1.06[b]	1.05[m]	1.26[c]
Mo	0.92	460	0.41	0.32[b]		0.42[c]
Ru	0.49	550	0.38	0.45[e]		
Hf	0.09	252	0.34	0.42[k]		
Ta	4.48	258	0.65	0.87[b]	0.69[n], 0.73[o]	0.86[c]
W	0.012	390	0.28	0.26[b]		
Re	1.69	415	0.46	0.76[e]		
Os	0.65	500	0.39	0.54[e]		
Ir	0.14	420	0.34	0.50[b]		
α-La	4.88	151	0.81[p]		(0.77)[q]	
β-La	6.00	139	0.93[p]			
Th	1.38	165	0.56[b]	0.52[b]		

From P. B. Allen, Handbook of Superconductivity, ed. C. Poole, Jr. (Academic, New York, 1999), Ch. 9, Sec. G, pp. 478-483.

TABLE IV. Values of λ for non-superconducting crystalline elements

Metal	λ_{tr}[a]	λ_{LDA}	λ_{other}
Li	0.35	0.45 – 0.51[b]	
Na	0.14		0.24[c]
K	0.11		
Rb	0.15		
Cs	0.16		
Cu	0.13	0.14[d]	0.14±0.02[e]
Ag	0.12		
Au	0.15		0.2[f]
Mg	0.20[g]		
Ca	0.05		
Ba	0.27		
Sc	0.51[g]		
Y	0.62[g]		
Pd	0.47	0.35[d]	
Pt	0.66		
Gd			0.6[h]

TABLE V. Values of λ for crystalline compounds and ordered intermetallics

Metal	T_c	λ_{tun}	λ_{tr}	λ_{McM}
In_2Bi	5.6	1.40[a]		
Bi_2Tl	6.4	1.63[a]		
Tl_7Sb_2	5.2	1.43[a]		
V_3Si	17.1	0.89[b]		
Nb_3Al	18.5	1.7[c]		
Nb_3Sn	17.8	1.75[d]		
Nb_3Ge	≈20	1.7[b]		
NbN	16.0	1.46[b]		
NbO	1.4		0.51[e]	0.41[e]
ReO_3	<0.02		0.35[f]	
RuO_2	<4.2		0.5 ± 0.1 [g]	
$CoSi_2$	1.22		0.44[f]	
Pd_2Si			0.15 – 0.20[f]	
$LuNi_2B_2C$	16.1		0.9[h], 0.8[i]	1.0[h]
$La_3Ni_2B_2N_{3-\delta}$	12.25		0.29[j]	0.86[j]

From P. B. Allen, Handbook of Superconductivity, ed. C. Poole, Jr. (Academic, New York, 1999), Ch. 9, Sec. G, pp. 478-483.

Strong Coupling: Good News, Bad News

P. B. Allen

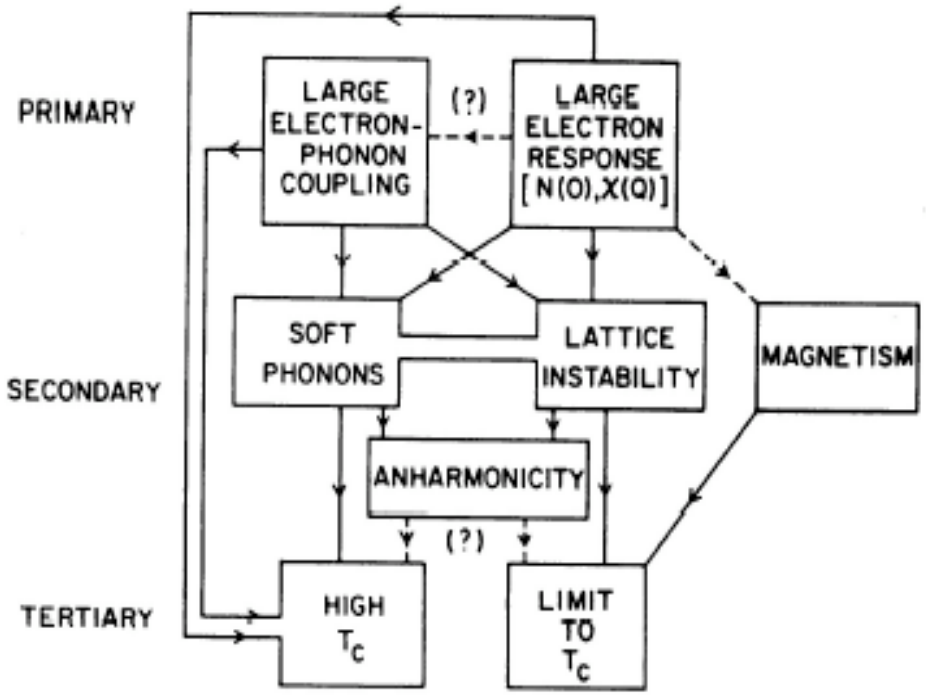


Fig. 3. Causative relations are indicated by arrows. High T_c is partly a direct consequence of the primary factors, and partly indirect through the phonon dispersion. Dashed lines with arrows represent less certain relationships.

Matthias' Rules (ca. 1970)

1. Must use transition metal atoms
2. Special e/a ratios [high values of $N(E_F)$]
3. Cubic symmetry is best

Unwritten Rules

1. Coupling must be uniform in q, not focused
2. Coupling to all phonon branches, not a few
3. Very soft phonons are not favorable

Superconductivity and Lattice Instability in Compressed Lithium: Fermi Surface Hot Spots

Warren E. Pickett,
Deepa Kasinathan, Jan Kunes,
Amy Lazicki, Helge Rosner,
Choong-shik Yoo and
Richard T. Scalettar

UC Davis

Acknowledgements to: S. Y. Savrasov,K. Koepernik, A. K. McMahan

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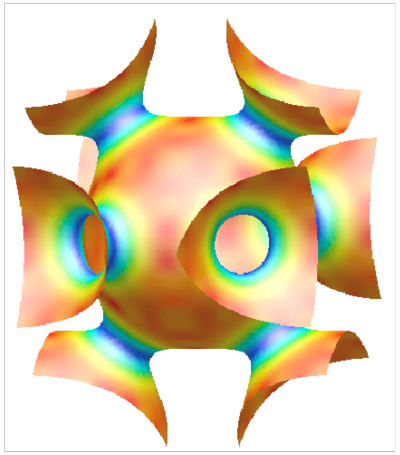
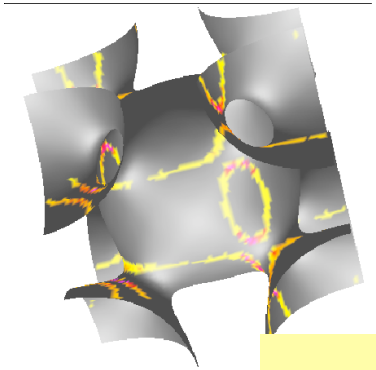
Pressure as a Tool to Produce Superconductors: Elemental Metals under Pressure: T_c=20-25K





Li: T_c up to 20 K

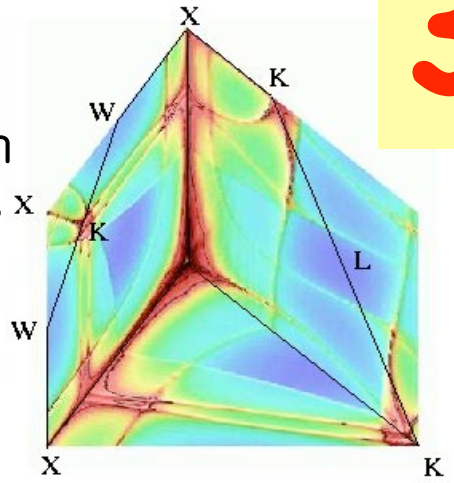
Y: T_c up to 20 K

Ca: T_c up to 25 K

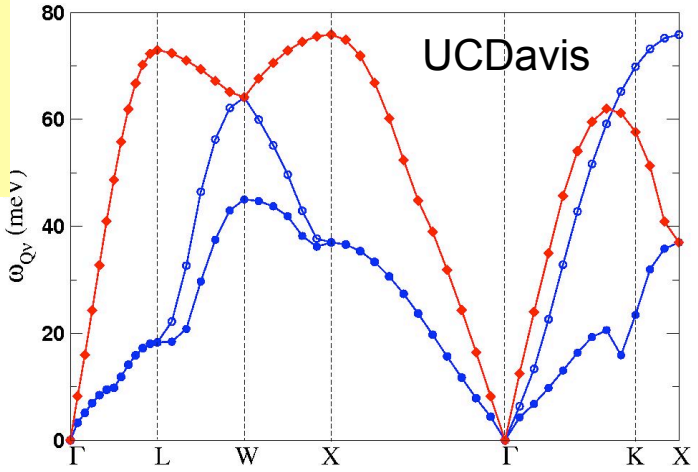
!

3D

Nesting function in three planes



Lithium

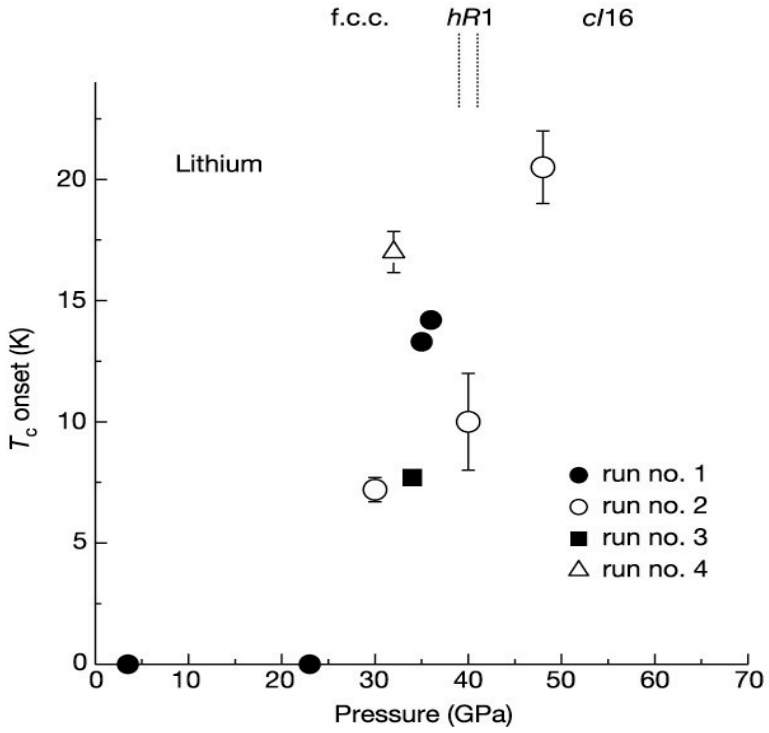


fcc Li: strong coupling, phonon anomalies, instabilities under pressure

$$\xi_{\vec{Q}} = \sum_k \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = V_c \int_{\mathcal{L}} \frac{d\mathcal{L}(k,Q)}{|\vec{v}_k \times \vec{v}_{k+Q}|}$$

“Superconductivity in Compressed Lithium at 20 K”

T_c vs. Pressure



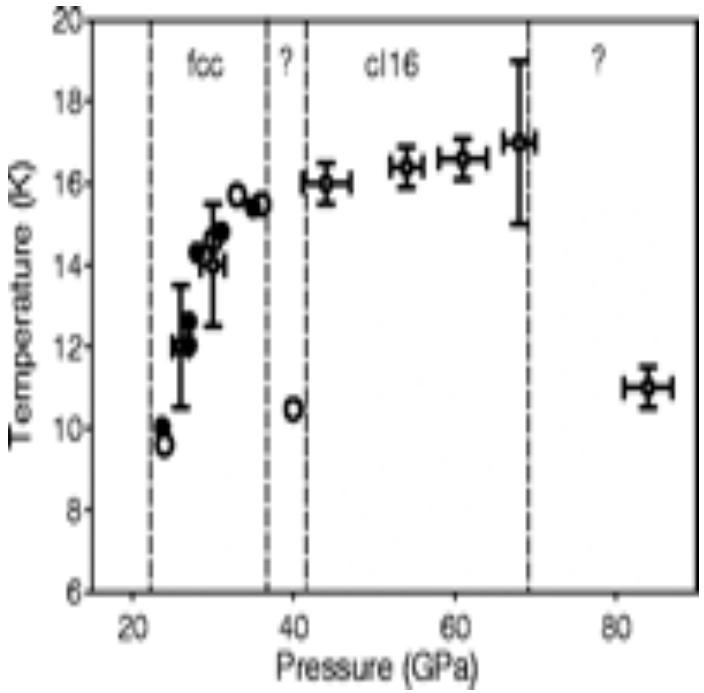
The initial report of superconductivity at elevated temperature in lithium

Shimizu et al.
Nature 419, 597 (2002).

Appearance of superconductivity above 30 GPa;
20 K at 50 GPa.

Quick Confirmation: Geophysical Lab

T_c vs. Pressure

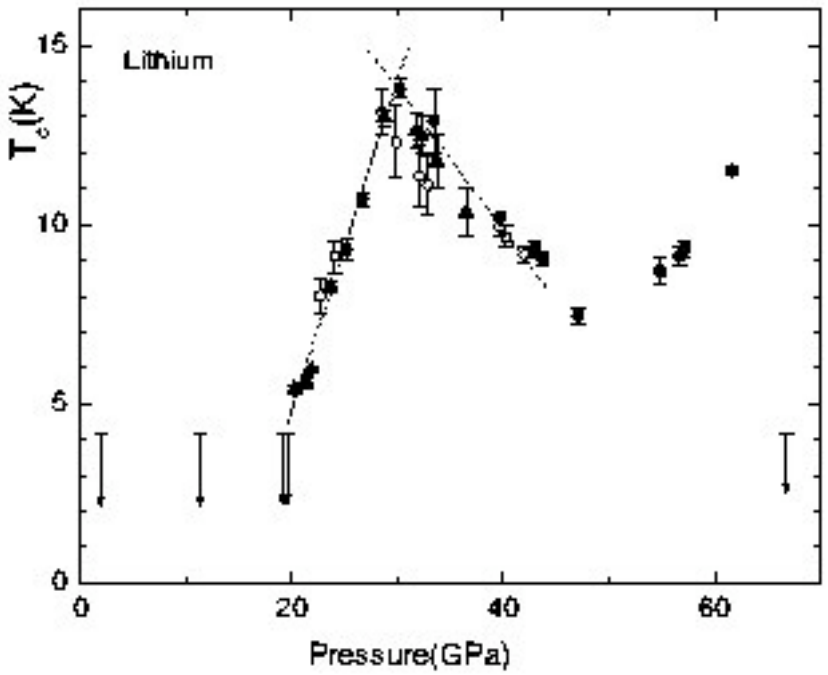


- **Struzhkin, Eremits, Gan, Mao, Hemley,**
- *Science 298, 1213 (2002).*

- **Superconductivity and**
- **identification of phases.**
- **T_c=16K in fcc phase**
- **around 40 GPa.**

Further elucidation: Washington University

T_c vs. Pressure

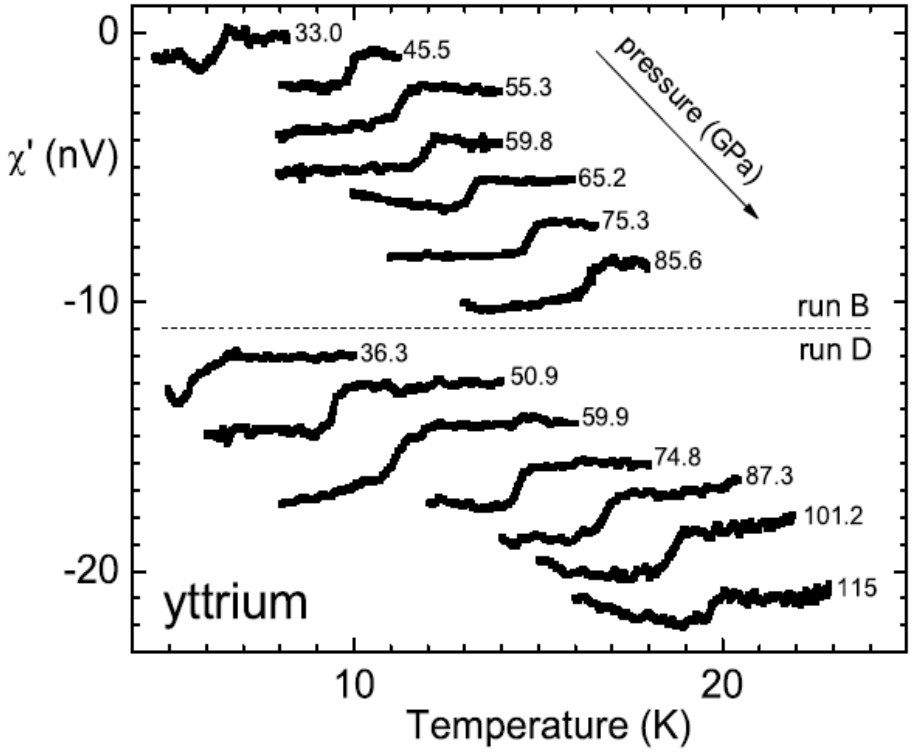


- **Deemyad and Schilling**,
- ***PRL 91, 167001 (2003).***

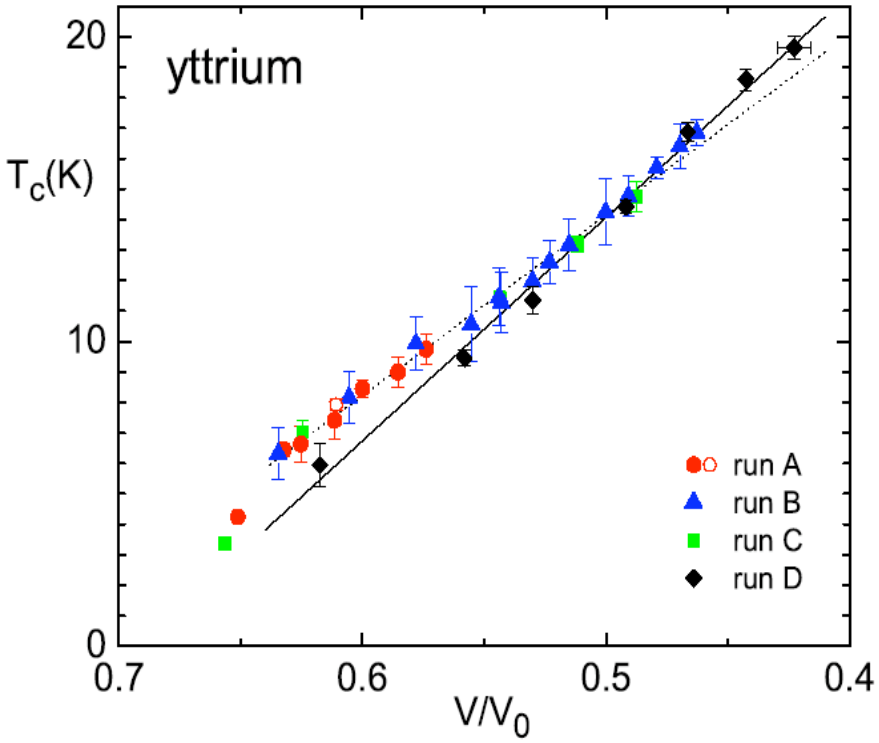
- **Superconductivity peak**
- **at 30 GPa in fcc phase**

- **Near-hydrostatic conditions**

- **Rise in Tc beyond 40 GPa.**



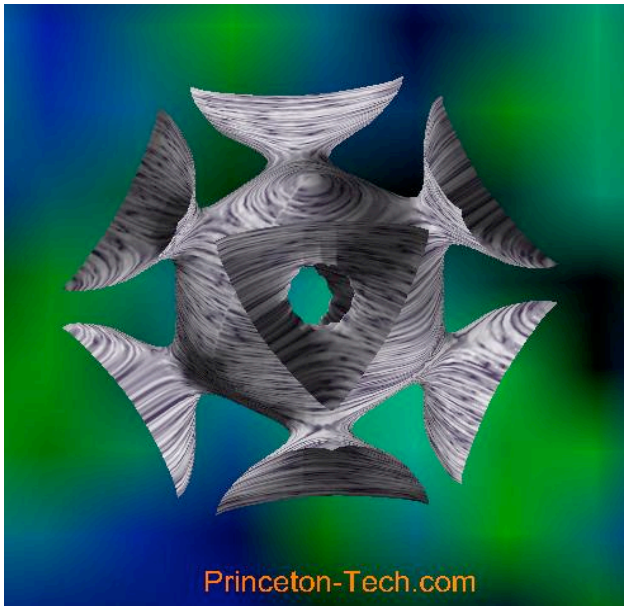
Real part of the ac susceptibility signal in nanovolts versus temperature for yttrium at a variety of different pressures ranging from 33 to 115 GPa.
J. J. Hamlin *et al.*, Phys. Rev. B **73**, 094522 (2006)
J. J. Hamlin *et al.,* unpublished (2006)



Results of experiments of *Tc* versus relative volume V/V0

Computational Methods

- **LAPW, FPLO codes for**
  - **study of change of**
  - **electronic structure**
  - **under pressure**



Savrasov's full potential LMTO code for calculation of:

•phonon dispersion curves

•el-ph matrix elements

•spectral function

Savrasov, PR B 54, 16470 (1996)

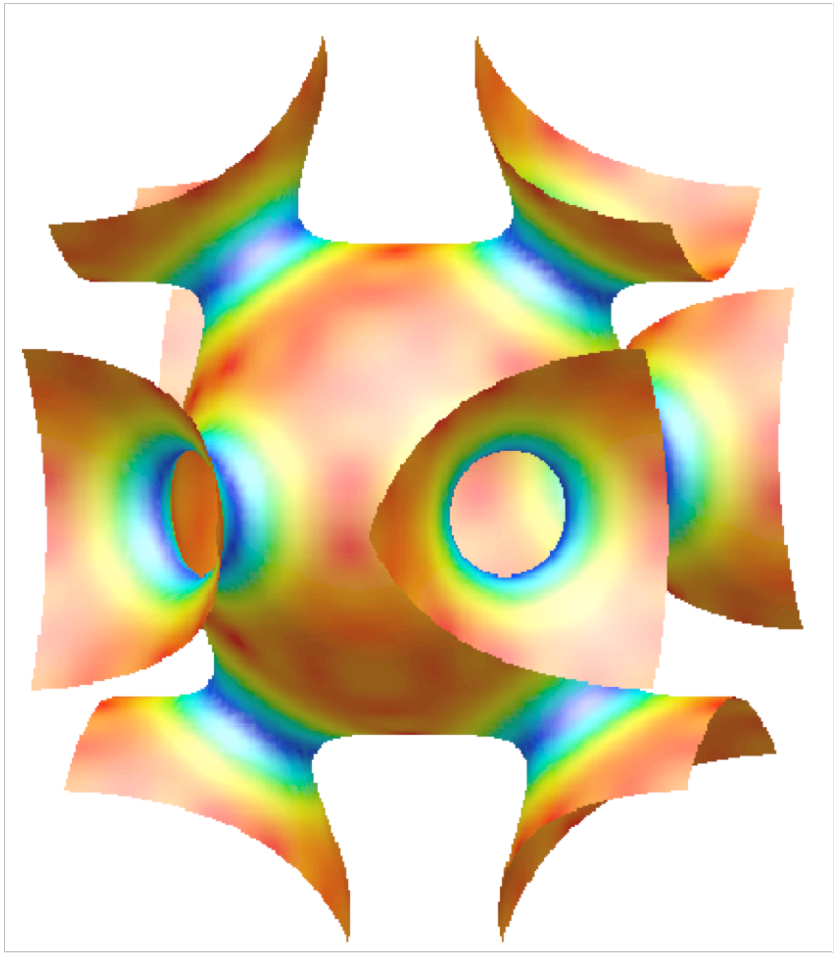
Savrasov & Savrasov, ibid. 16487 (1996)

Some Basic Orientation

- **Fermi surface of Li in fcc structure at 35 GPa**
- **(V/Vo = 0.51)**

- **Necks appear along <111> directions**
- **(a la Cu) at 20 PGa**

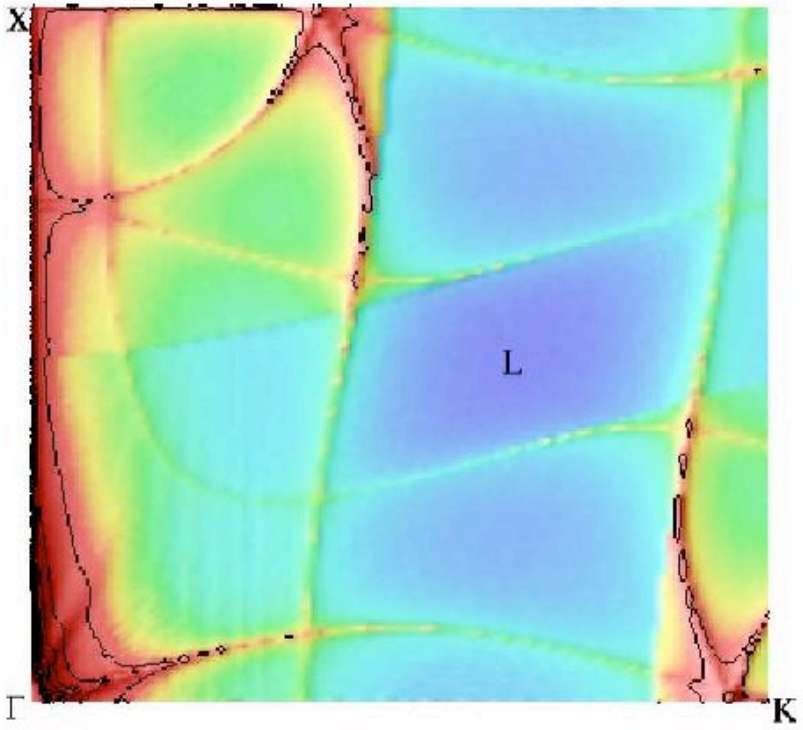
- **Velocities: 0.3 on necks, 0.7 on bellies (10^8 cm/s)**



The Nesting Function in fcc Li

$$\xi_{\vec{Q}} = \sum_{k} \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = V_c \int_{\mathcal{L}} \frac{d\mathcal{L}(k,Q)}{|\vec{v}_k \times \vec{v}_{k+Q}|}$$

G–K–L–X plane

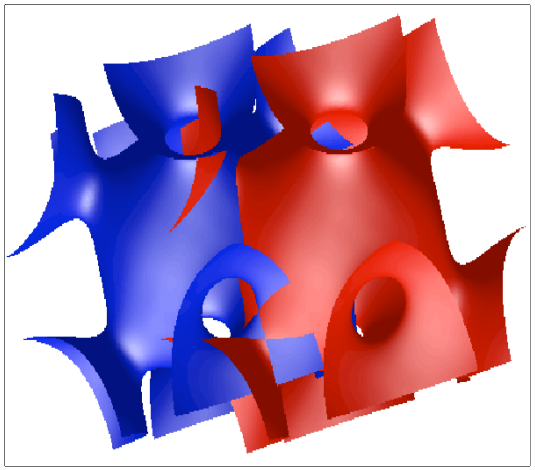


For spherical Fermi surface, there would be only step discontinuities. Some can be seen: blue to green across ridge.

Red regions are mountain ranges, which contain strong weight and can be logarithmically divergent.

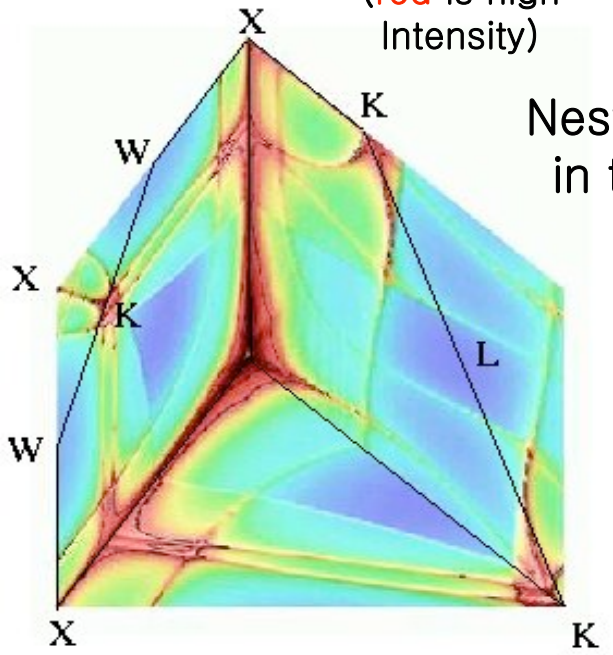
Fermi Surface Nesting Function for Li (35 GPa)

Intersection of Fermi surface (Q=0)
With Fermi surface at Q=0.71(1,1,0)

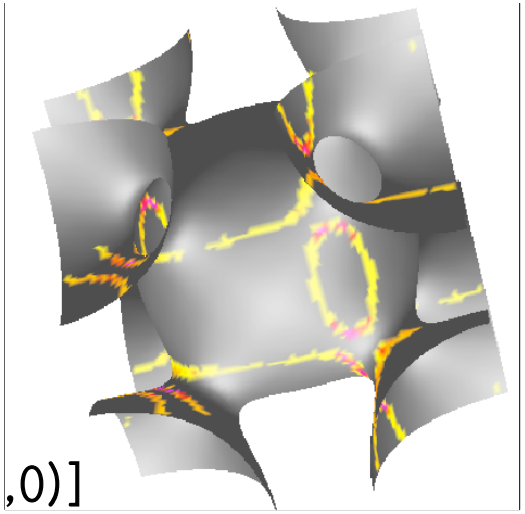


$$\xi_{\vec{Q}} = \sum_k \delta(\varepsilon_k)\delta(\varepsilon_{k+Q}) = V_c \int_{\mathcal{L}} \frac{d\mathcal{L}(k,Q)}{|\vec{v}_k \times \vec{v}_{k+Q}|}$$

(red is high Intensity)



Nesting function in three planes



Hot spots (yellow) arising from the intersection shown above [Q=0.71(1,1,0)]

Electron-Phonon Spectral Function

Evolution of el-ph coupling weight with pressure

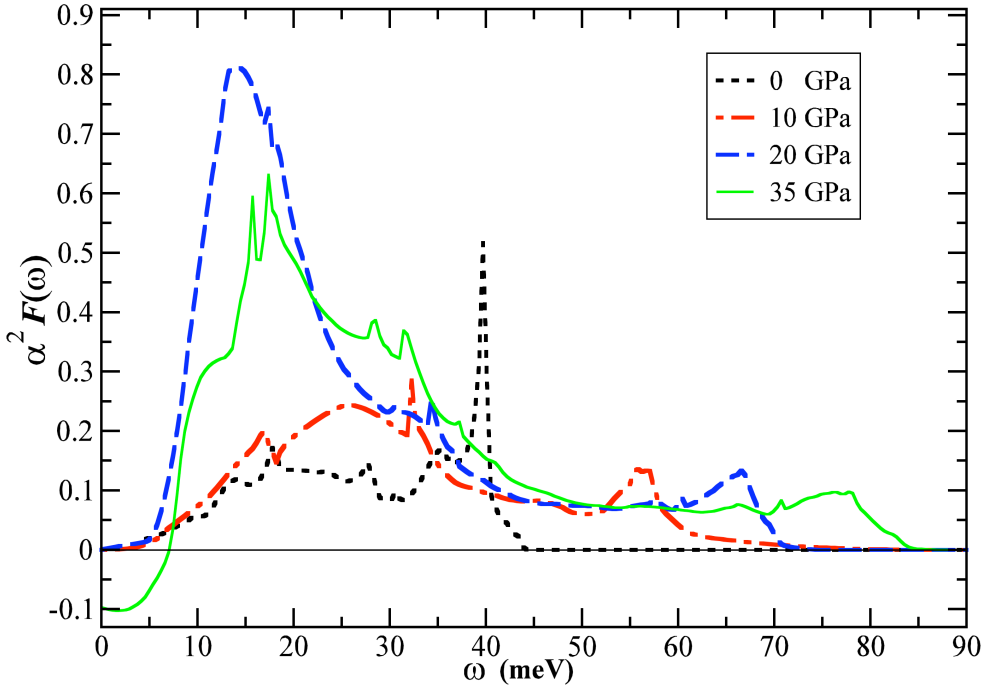
P=0: weak, evenly spread

P=10: LA mode hardens, weight grows at 30 meV

P=20: LA mode is harder, large weight at 15 meV

P=35: instability (see low frequency region)

El-ph weight grows at low energy (not high as in MgB2)



Material Constants from the Spectral Function

P (GPa)	a (a_B)	V/V_0	$N(E_F)$ (states/Ry/spin/atom)	$\langle\omega\rangle$ (meV)	$\langle\omega^2\rangle^{1/2}$ (K)	ω_{ln} (K)	λ
0	8.0069	1.00	3.537	21	278	209	0.42
10	7.2298	0.74	3.031	22	229	225	0.65
20	6.8003	0.61	2.789	10	170	84	3.15
35	6.4085	0.51	2.573	10	220	130	2.77

Calculating T_c supposing that $\mu^*=0.15$, one obtains

P= 0: T_c = 0.4 K

P=10: T_c= 5 K

P=20: T_c= 20 K

Clearly these numbers are not really accurate. Anharmonic corrections will become large, when phonons begin to become soft/unstable .

Summarizing Comments on Lithium

- **Band structure evolves strongly under pressure: change from s metal to sp metal. Not a very striking change, however.**
- **Fermi surface in fcc structure develops necks along the (111) directions. Distortion from spherical seems to be significant.**
- **On-Fermi-surface scattering processes become focused onto certain "hot spots" near the necks.**
- **Linear response calculations of EPI indicate strong coupling and T_c ~ 15-20 K, consistent with experiment.**
- **But: we have no simple physical picture of the strong coupling. And yttrium and calcium also have T_c ~ 20-25K under pressure.**

Y, Ca: also “high T_c” under pressure

- Y: 20 K around 1 GPa, still increasing
- Ca: 25 K reported above 1 GPa
- Ca: structures and structural transitions under pressure are unusual, interesting

Electron-Phonon Coupling in 2D

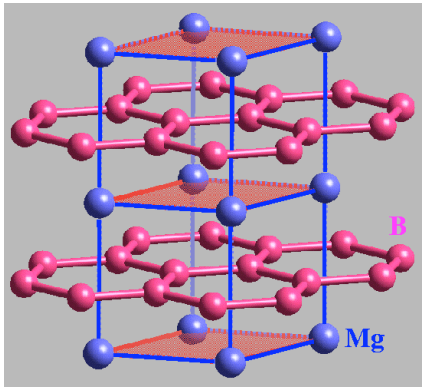
The remarkable case of MgB_2:
unconventional el-ph coupling.

Akimitsu's Discovery: 2001

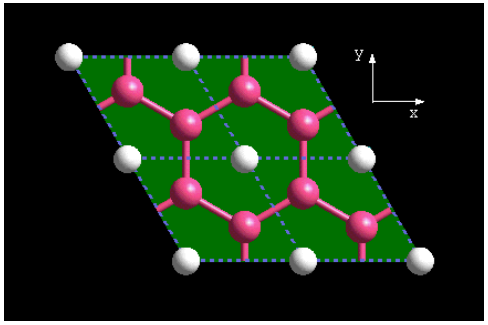
MgB_2, a common chemical reagent.

2D

Searching for ferromagnetism, superconductivity at 40 K was discovered



Quickly reproduced and synthesis techniques were extended by several groups

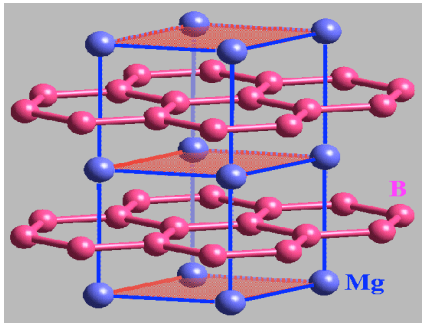


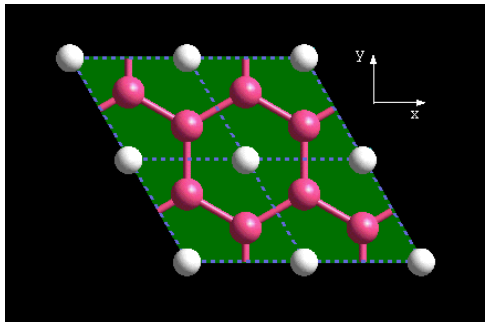
Crystal structure is simple. Quasi-2D.

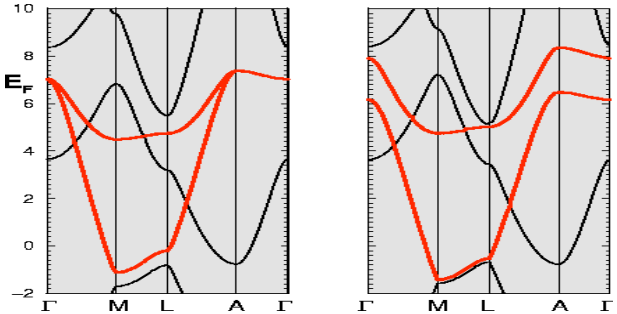
Electronic structure is simple: s-p electrons.

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

Four Months Later: Puzzle Solved!







T. Yildirim (NIST)

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…….

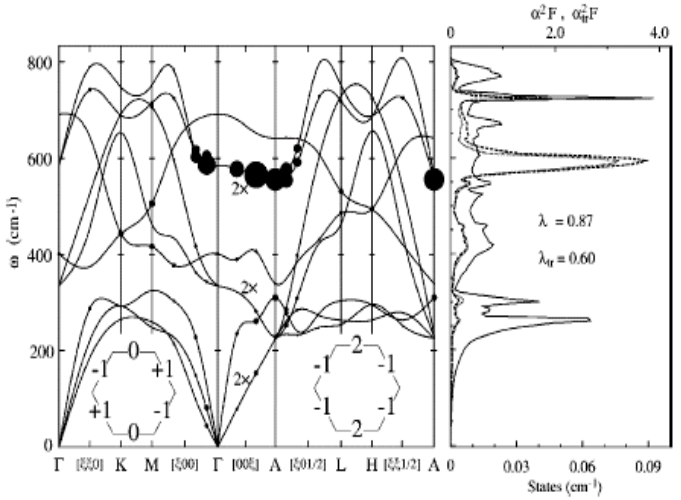


FIG. 1. Left: Calculated phonon dispersion curves in MgB_2. The area of each circle is proportional to the mode λ. The insets at the bottom show the two Γ*A* *E* eigenvectors (not normalized), which apply to the holes at the top of the σ bands (bond-orbital coefficients) as well as to the optical bond-stretching 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.

Electron-Phonon Coupling: General Results for $\lambda_{Q\nu}$ and $\gamma_{Q\nu}$

P. B. Allen, PR B6, 2577 (1972)

$$\lambda = \frac{1}{N_\nu}\sum_{Q,\nu=1}^{N_\nu}\lambda_{\vec{Q},\nu} = 2\int\frac{\alpha^2F(\omega)}{\omega}d\omega$$

$$\alpha^2F(\omega) = \frac{2}{\pi N(0)\omega}\sum_{Q\nu}\gamma_{Q\nu}\delta(\omega_{Q\nu}-\omega)$$

$$\omega_{Q\nu}^2 = \Omega_{Q\nu}^2 + 2\Omega_{Q\nu}^2 Re\ \Pi(Q,\omega_{Q\nu})$$

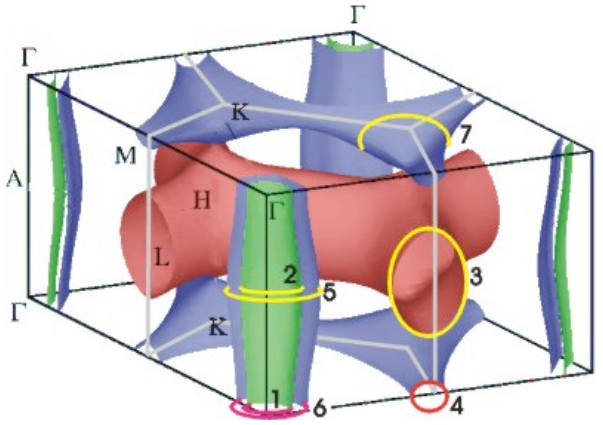
$$\gamma_{Q\nu} = \frac{\Omega_{q\nu}}{\omega_{Q\nu}} Im\ \Pi(Q,\omega_{Q\nu})$$

$$= \pi\sum_k |M_{k,k+Q}|^2\delta(\varepsilon_k)\delta(\varepsilon_{k+Q})$$

$$\lambda = \frac{1}{N_\nu}\sum_{Q\nu}\lambda_{Q\nu} = \frac{4}{\pi N(0)}\sum_{Q\nu}\frac{\gamma_{Q\nu}}{\omega_{Q\nu}^2}$$

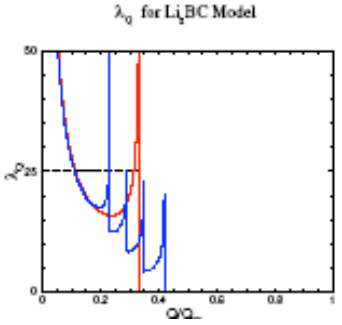
3% of phonons have $\lambda \sim 25$!

Rest of phonons have $\lambda \sim 0.3$



$$\lambda_{\vec{Q},\nu} = 4\frac{2}{\omega_{\vec{Q},\nu}}\sum_k |M_{k,k+Q}|^2\delta(\varepsilon_k)\delta(\varepsilon_{k+Q})$$

$$= 4\frac{4\pi V_c|M|^2}{\omega_{\vec{Q},\nu}ck_F^2}\frac{1}{x\sqrt{1-x^2}}, x \equiv \frac{Q}{2k_F}$$



Phonons and Electrons in 2D

Reference system ("unrenormalized") → renormalized system

Limits to Strong Coupling in 2D

2D MgB_2-like material, circular Fermi surfaces

$$\omega_{Q\nu}^2 = \Omega_{Q\nu}^2 + 2\Omega_{Q\nu}\Pi(Q,\omega_{Q\nu})$$

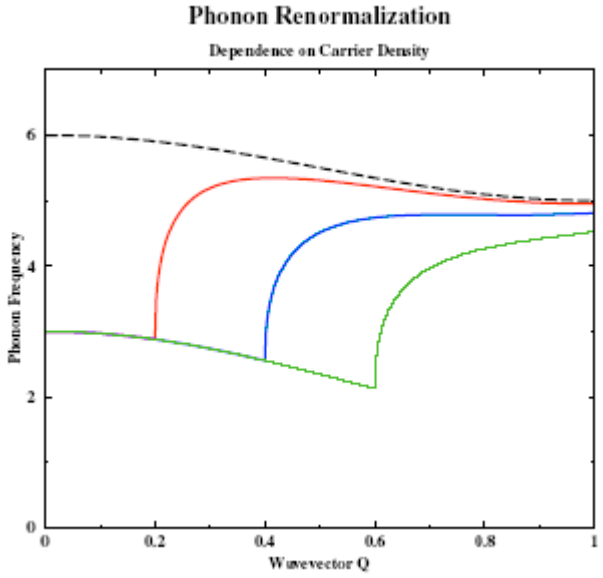
$$\Pi^\sigma(Q,\omega) = -2\sum_k |g_{k,Q}|^2 \frac{f_k - f_{k+Q}}{\varepsilon_{k+Q} - \varepsilon_k - \omega - i\delta},$$

$$\Re e\ \Pi^\sigma(Q,\omega_Q) \approx -2|g|^2 N(0) d_b^2 \hat{\chi}_L^{2D}(Q),$$

$$\hat{\chi}_L^{2D}(Q) = \theta(1-\eta_Q) + \left[1 - \sqrt{1-\eta_Q^{-2}}\right]\theta(\eta_Q - 1)$$

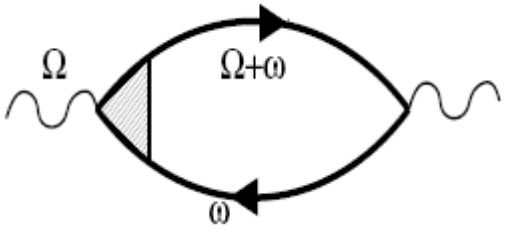
$$\eta_Q \equiv \frac{Q}{/2k_F}, \quad |g|^2 = \frac{\mathcal{D}^2}{2M\Omega}$$

$$\frac{\omega_Q^2}{\Omega_Q^2} = 1 - d_b^2 \frac{m^*}{2\pi}\frac{\mathcal{D}^2}{M\Omega_Q^2}, \quad Q < 2k_F$$



Magnitude of renormalization is independent of carrier density

Phonon Renormalization (Self Energy)



Cylinder Fermi surface leads to sharp Kohn anomaly

Large matrix elements lead to strong renormalization for $Q<2k_F$

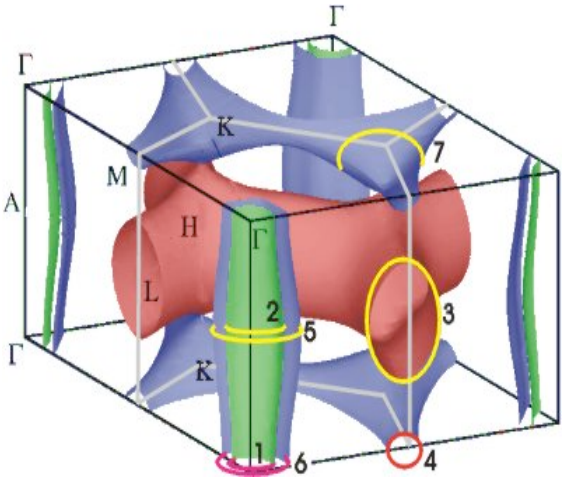
Extreme Electron-Phonon Coupling: Kohn Anomalies

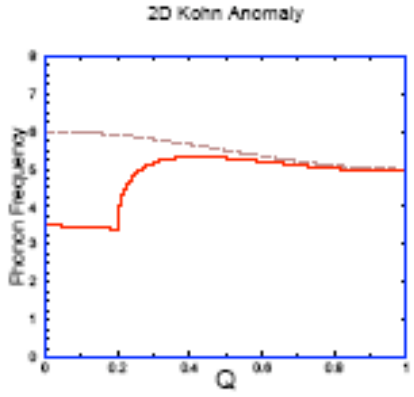
$$\omega_{Q\nu}^2 = \Omega_{Q\nu}^2 + 2\Omega_{Q\nu}^2 \Pi(Q, \omega_{Q\nu})$$

$$\Pi(Q,\omega) = -2\sum_k |M_{k,k+Q}|^2 \frac{f_k - f_{k+Q}}{\varepsilon_{k+Q} - \varepsilon_k - \omega - i\delta}$$

2D dispersion, slowly varying matrix elements give

$$\Pi_\nu(Q,\omega) = -2|M_\nu|^2 \chi_L^{2D}(Q,\omega)$$





Pinpointing of Strong Electron-Phonon Coupling

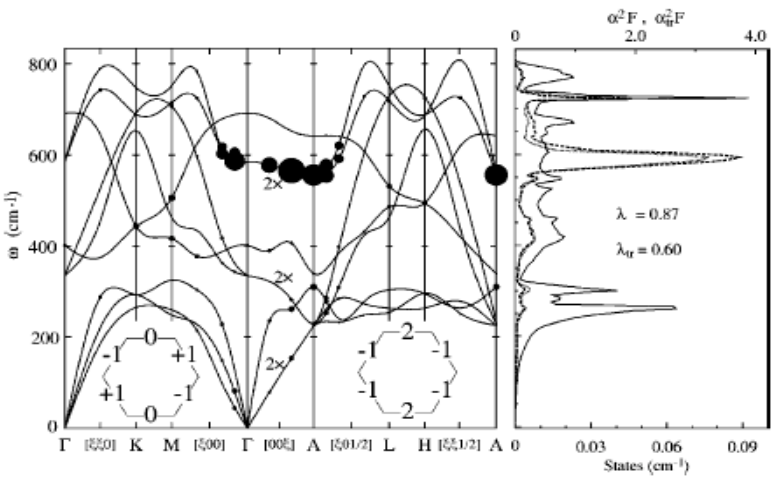
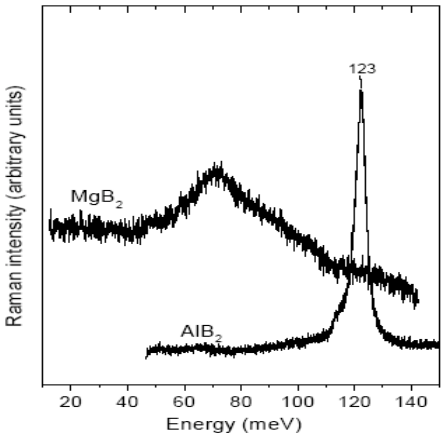
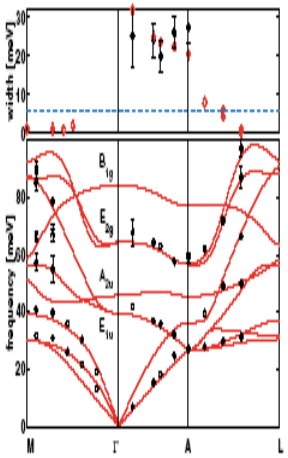


FIG. 1. Left: Calculated phonon dispersion curves in MgB_2. The area of each circle is proportional to the mode λ. The insets at the bottom show the two ΓA E eigenvectors (not normalized), which apply to the holes at the top of the σ bands (bond-orbital coefficients) as well as to the optical bond-stretching 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.



Raman spectrum
Bohnen, Heid, Renker (2002)



Shukla et al. Phys. Rev. Lett. (2003)
Inelastic x-ray scattering measurements

3% of phonons have $\lambda \sim 25$!
Rest of phonons have $\lambda \sim 0.3$

W. Weber et al.,
PRL (1978)

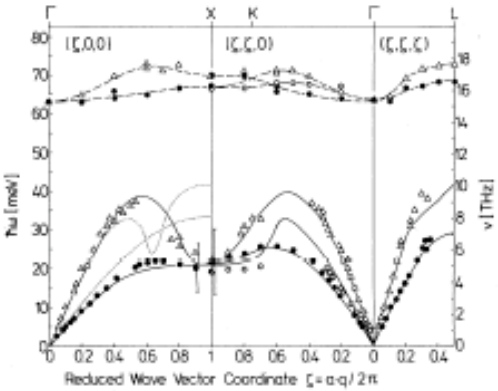
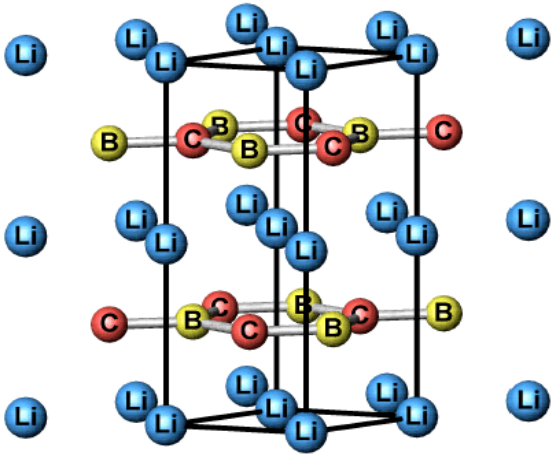


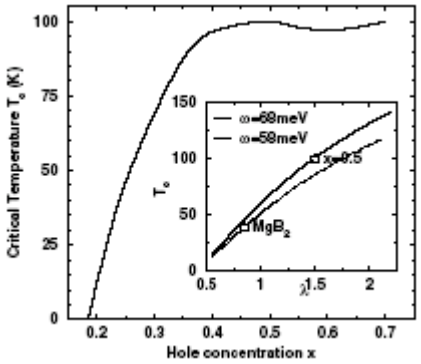
FIG. 1. Phonon dispersion curves for $VN_{0.86}$ (open

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 (or higher) might be possible



Not so simple experimentally!

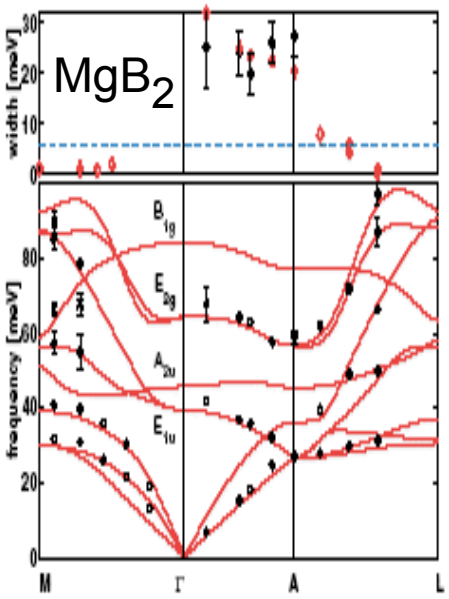
Several reports of inability to prepare $Li_{1-x}BC$
Reports that $Li_{1-x}BC$ is not superconducting:

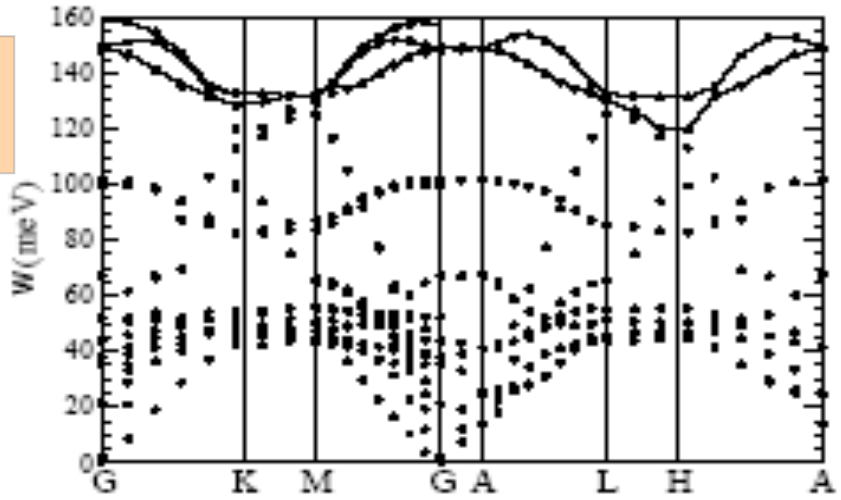
Zhao, Klavins, Liu, J. Appl. Phys. (2003)
Fogg, Claridge, Darling, Rosseinsky (2003)

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

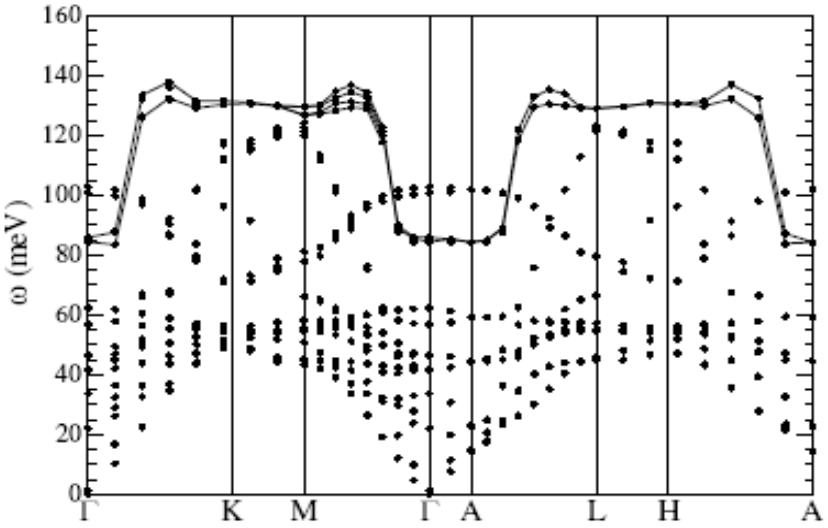
Electron-Phonon Coupling Strength Calculated for $Li_{1-x}BC$

Semiconductor x=0
Simple vibrational spectrum





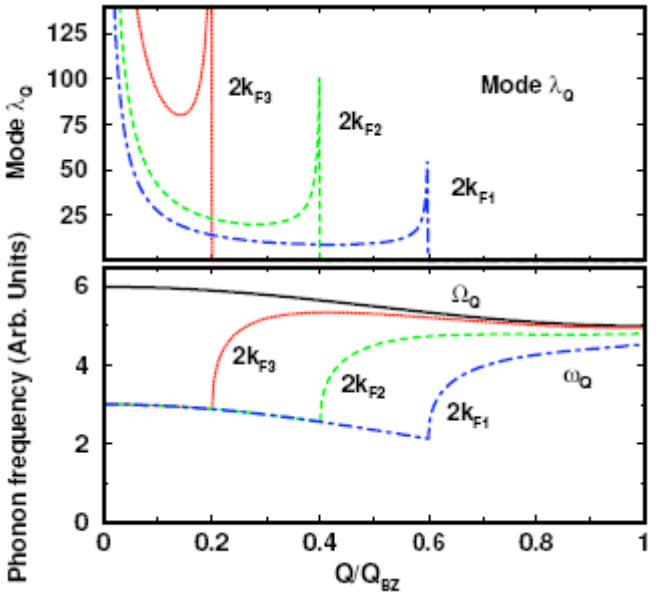
Metal for x=0.25
Extreme Kohn anomalies



EI-Ph Coupling in MgB_2-like Systems

Mode λ_Q and Total Coupling Strength λ

$$
\begin{aligned}
\lambda_Q &= \frac{2}{\pi N(0)} \frac{\gamma_Q}{\omega_Q^2} \\
\gamma_Q &= \pi \Omega_Q |g|^2 [N(0)]^2 d_b^2 \hat{\xi}(Q), \\
\hat{\xi}(Q) &= \frac{\sum_k \delta(\varepsilon_k)\delta(\varepsilon_{k+Q})}{[\sum_k \delta(\varepsilon_k)]^2} = \frac{A_{BZ}}{A_{FS}} \frac{1}{\pi} \frac{\theta(1-\eta)}{\eta\sqrt{1-\eta^2}} \\
\lambda &= \sum_{Q\nu} \lambda_{Q\nu} = d_b^2 \frac{N(0)\mathcal{D}^2}{M\omega_Q^2} \leftrightarrow \frac{N(\varepsilon_F) < I^2 >}{M < \omega^2 >} \\
&= \frac{d_b^2 N(0)\mathcal{D}^2}{M\Omega_Q^2 - d_b^2 N(0)\mathcal{D}^2}, \quad N(0) = \frac{m^*}{2\pi} \\
&= \frac{\lambda_o}{1-\lambda_o}, \quad \lambda_o \equiv \frac{d_b^2 N(0)\mathcal{D}^2}{M\Omega_Q^2}
\end{aligned}
$$



- mode λ_Q *scales inversely with carrier density* ($A_{FS} \equiv \pi k_F^2$)
- total λ is independent of carrier density

Why Isn't MgB_2 a Higher T_c Material?

How could MgB_2 have been better? Relations to use:

$$\lambda_o \equiv \frac{d_b^2 N(0)\mathcal{D}^2}{M\Omega^2}; \quad \lambda = \frac{\lambda_o}{1-\lambda_o}$$

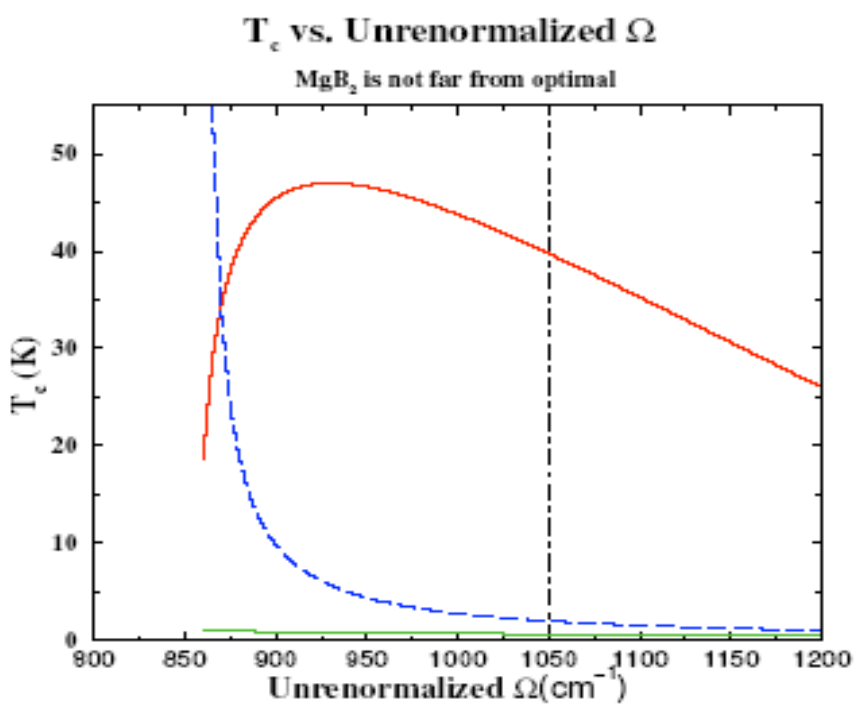
$$T_c \approx \frac{<\omega>}{4}[e^{2/\lambda_{eff}} - 1]^{-1/2}; \quad \lambda_{eff} = \frac{\lambda - \mu^*}{1 + 0.75\lambda\mu^* + 2\mu^*}$$

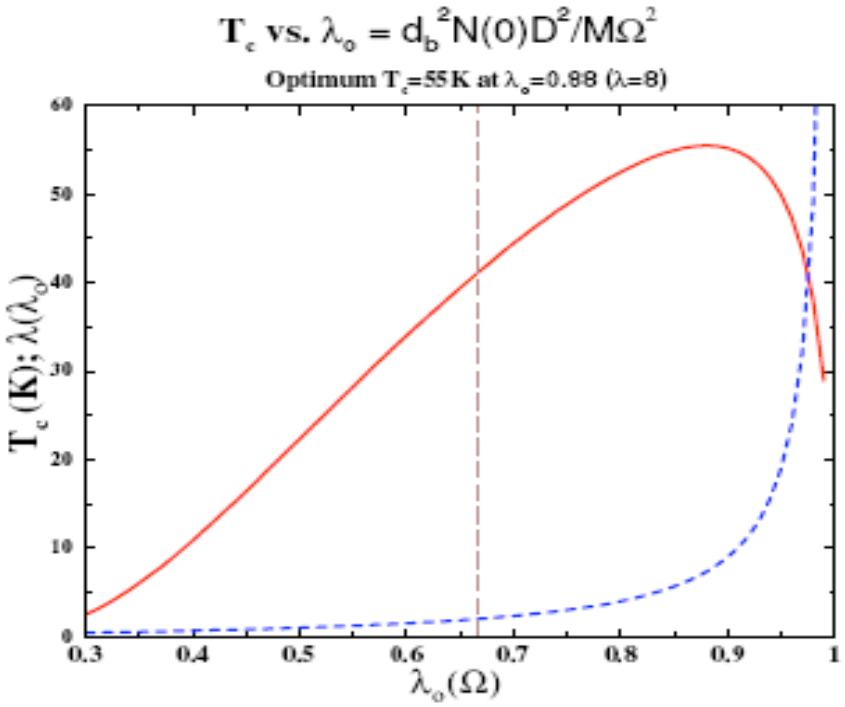
• Suppose Ω had been different from what it is, Ω_{AlB_2} =1050 cm^{-1}. With other factors the same, the parent system would have been unstable if $\Omega = 850$ cm^{-1}. Hence MgB_2 is not so far from not having existed.

• What if Ω were even bigger? λ_o and λ would be smaller but the energy/temperature scale (prefactor in T_c) would have been higher.

• What if the coupling (deformation potential $\mathcal{D}$) had been larger? If $\mathcal{D}$) were 20% larger ($\mathcal{D}^2$ 44% larger), $\lambda_o \to 1$ and MgB_2 would be unstable.

Engineering an Optimized MgB_2





An Optimized MgB_2 would have T_c=55-60K

Is there some other way to win?

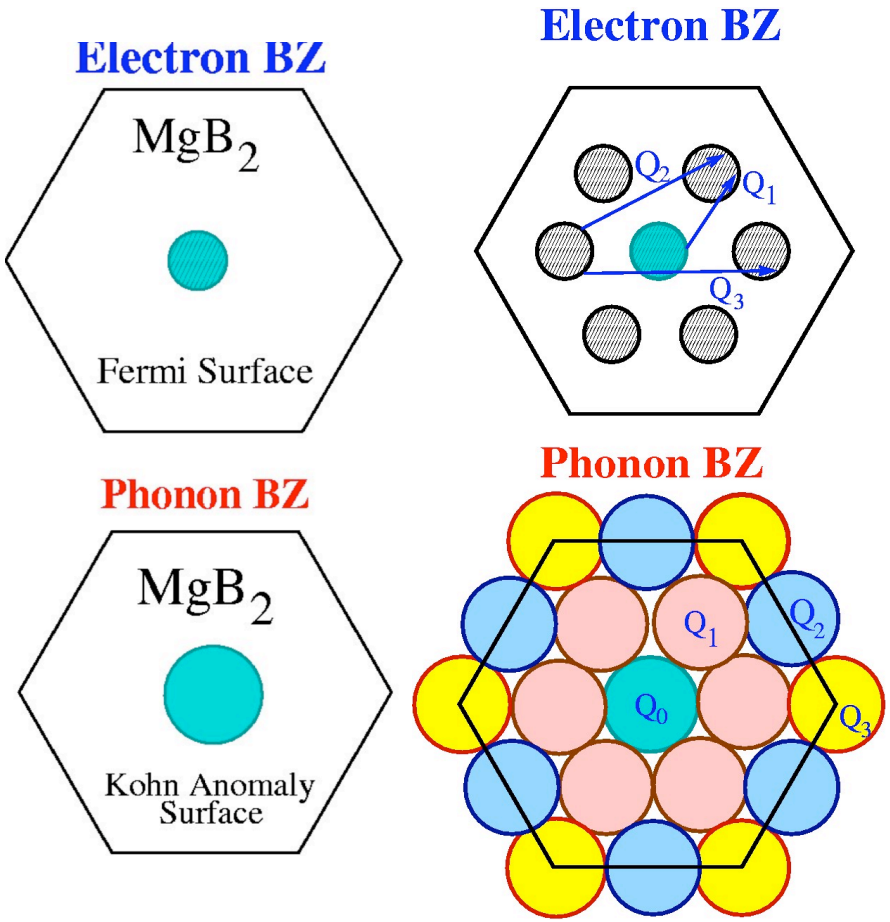
Yes.

Make serious use of
two-dimensionality in the boson coupling.

Design of higher T_c superconductors: is it viable?

Rational Design/Search for new hTS

Example of one design criterion



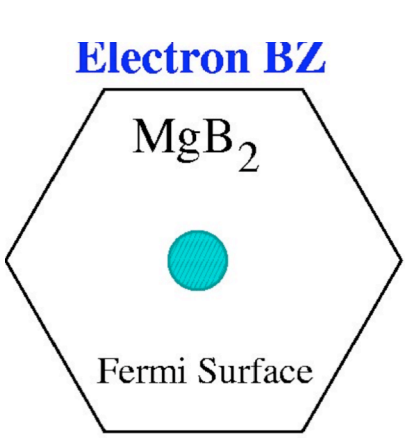
Select band structure to enable the phonons to use more of the Brillouin zone

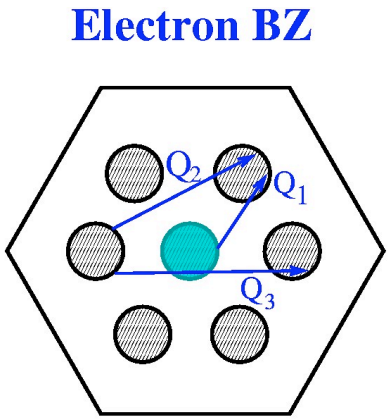
Design of higher T_c superconductors: is it viable?

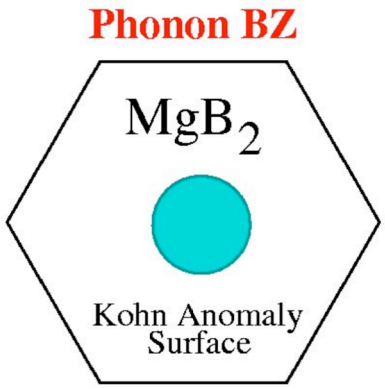
Rational Design/Search for new hTS

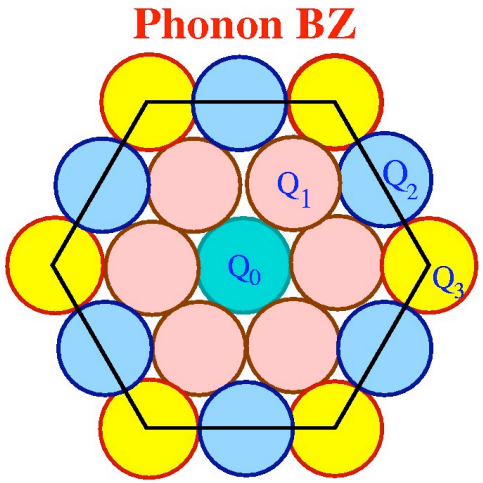
Rational design of 2D superconductors with substantially increased is viable.

Select band structure to enable the phonons to use more of the Brillouin zone









Summarizing Comments

- Simple metals Y, Ca, and early transition metal Y become “high temperature” superconductors (20-25K) at high pressure. Strong coupling Eliashberg theory works for these metals, but there is no straightforward physical picture for why the coupling gets so large.

- MgB2 is an impressive el-ph superconductor in spite of using only 3% of its phonons effectively. This is a humbling lesson, and it provides a blueprint for even better superconductors in this class.