High Temperature Superconductivity in Hydrides

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Condensed Matter Seminar

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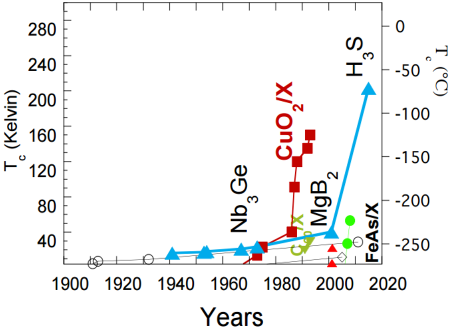
OUTLINE

-New T_c record in Sulfur Hydride system at extreme pressure
$T_c \approx 200K$, $P \approx 150GPa$ (Drozdov et al, Nature 2015)



THEORETICAL NEEDS

-Describe P-T phases and transitions of metallization (Enthalpy)
-Find electron and phonon dispersions (Density of States
-Develop T_c calculation (Eliashberg, McMillan-Dynes-Allen)

BACKGROUND

High T_c

Metallic Hydrogen: A High-Temperature Superconductor?
N. W. Ashcroft, Phys. Rev. Lett. 21, 1748 (1968)

Hydrogen Dominant Metallic Alloys: High Temperature Superconductors?
N. W. Ashcroft, Phys. Rev. Lett. 92, 187002 (2004)

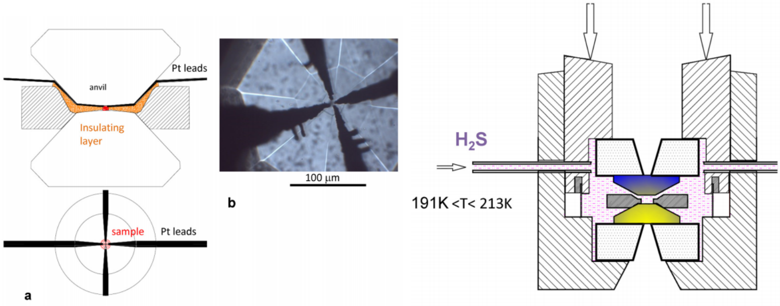
H_2S

"No experimental studies of hydrogen sulphide are known above 100 GPa"
Drozdov et al, Nature 2015

"Metallization and superconductivity in sulfur hydride occur at such high pressure when nothing is known in advance regarding the basic physical properties of the material under study. Not even the chemical formula is known and it is for theory to establish, in the first place, the very composition of the compound under investigation at such pressure."
Gorkov, Kresin, arXiv:1511.06926

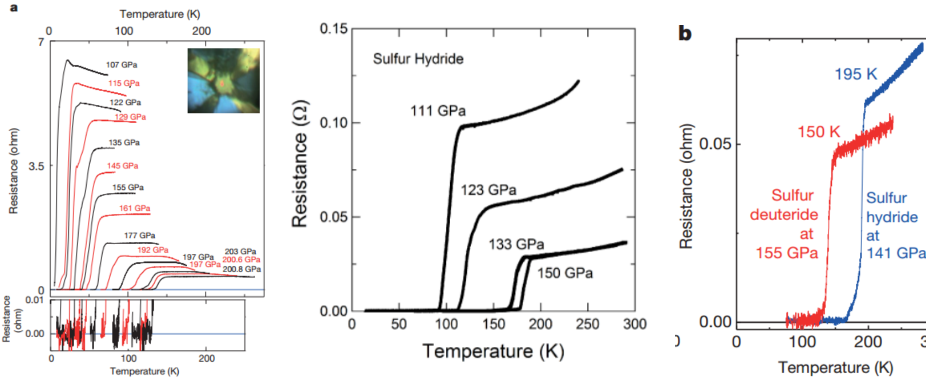
EXPERIMENT

Confirmed by TWO groups, Drozdov et al and Einaga et al, arXiv:1509.03156



Drozdov et al, Nature 2015
https://vimeo.com/131914556

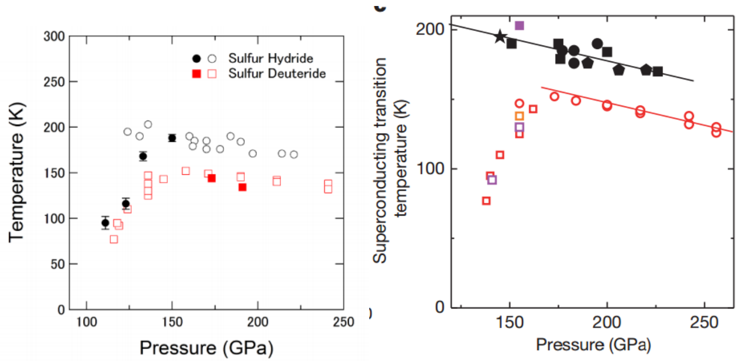
RESISTIVITY and ISOTOPE EFFECT



Drozdov, Eigana, Drozdov

-Annealing sample resulted in higher T_c and more stable measurements

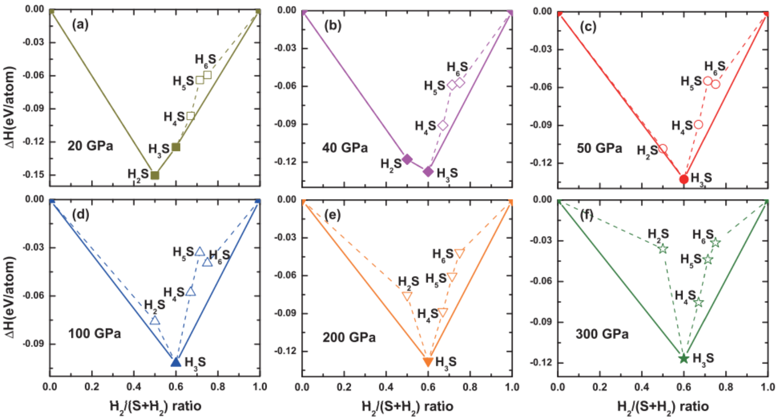
CRITICAL TEMPERATURE



Eigana, Drozdov

$T_c = 10 - 25K$ $(P = 100 - 250GPa)$ for elemental Sulfur

H_2S DECOMPOSITION

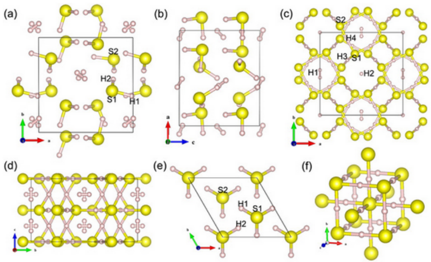


Duan et al, Scientific Reports 4, Article number: 6968 (2014)

$$3H_2S \rightarrow 2H_3S + S$$

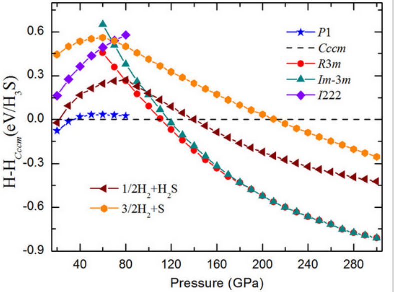
METALLIZATION

Figure 1: High-pressure crystal structures of $(H_2S)_2H_2$.

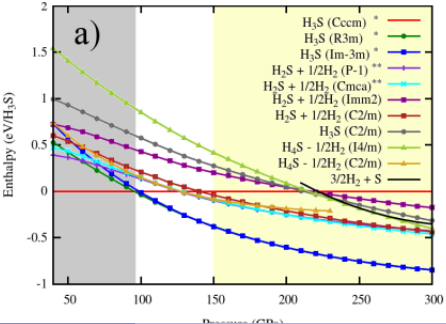


(a) P1 structure normal to the (001) plane, (b) P1 structure normal to the (010) plane, (c) *Cccm* structure normal to the (001) plane, (c) *Cccm* structure normal to the (100) plane, (e) *R*3*m*, and (f) *Im*−3*m*. Large spheres represent S and small spheres denote H atoms, respectively.

Duan

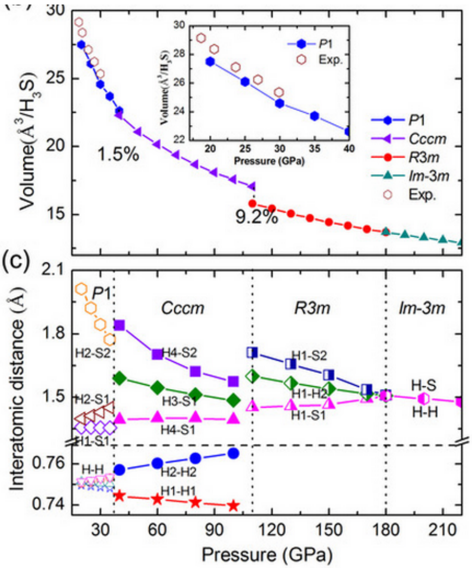


Duan



Flores et al, arXiv:1501.06336

METALLIZATION



General picture of phase transitions $P1 \rightarrow Cccm \rightarrow R3m \rightarrow Im-3m$ is unified among theories and agrees with XRD data (Eigana), but order of $R3m \rightarrow Im-3m$ is still under debate (See Gorkov paper)

-Flores

T_c CALCULATION

Allen and Dynes Phys. Rev. B 12, 905 (1975)

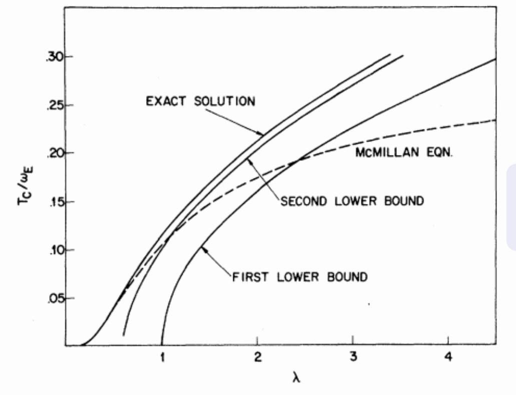
-Using an Einstein phonon spectrum T_c has *Lower* bound

$T_c > \frac{\omega_E}{2\pi}\sqrt{\frac{\lambda}{1+2\mu^*} - 1}$

$\lambda = 2\int d\omega\ \alpha^2(\omega)F(\omega)/\omega$

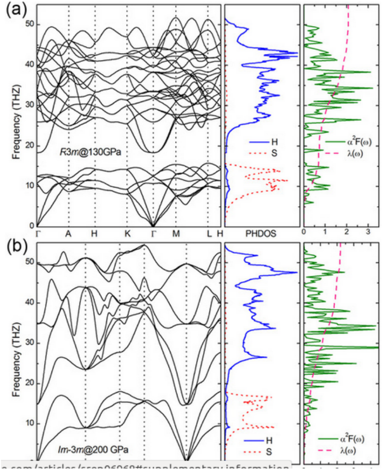
$\alpha^2(\omega)F(\omega)$ from phonon dispersion

$\mu^* \approx 0.1 - 0.15$ Coulomb pseudo-potential

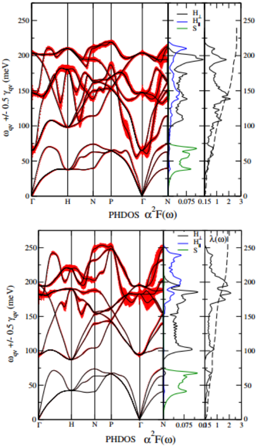


Larger $\lambda \Rightarrow$ Larger T_c/ω_E
Larger $\omega_E \Rightarrow$ Larger T_c

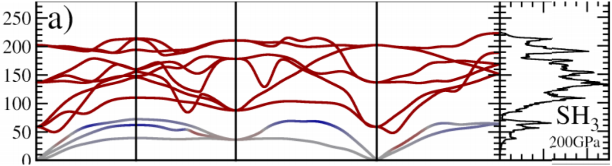
T_c CALCULATION PHONONS



Duan



Errea, PRL 114 (2015)



Flores

meV scale, $(\Gamma, N, H, \Gamma, P)$, $\alpha^2 F$

T_c CALCULATION PHONONS REVISITED

$$\Delta(\omega_n)Z = -2T\sum_m \int d\xi d\omega \frac{\alpha^2(\omega)F(\omega)}{\omega} D(\omega, \omega_n - \omega_m)\frac{\Delta(\omega_m)}{\omega_m^2+\xi^2}$$

$D(\omega, \omega_n - \omega_m) = -\frac{\omega}{[(\omega_n-\omega_m)^2+\omega^2]}$ Phonon Propagator

$Z \approx 1 + \lambda$ from renormalized mass

McMillan-Dynes-Allen

-Used by Duan, Flores, Errea

-replace ω in D with average $\tilde{\omega}_E$

-ok for *single low frequency* phonon contribution λ_E

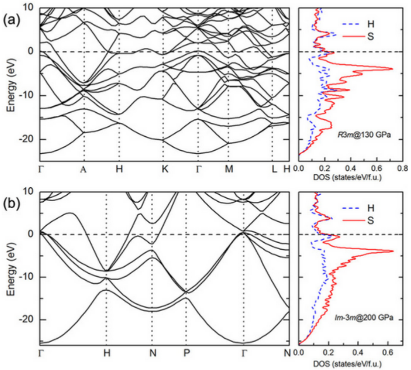
Proposed by Gorkov

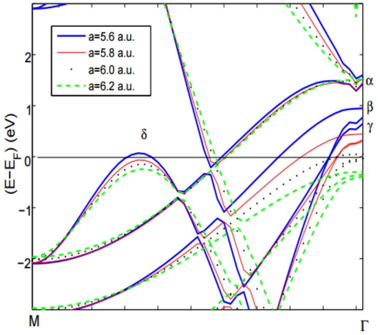
-replace ω in D with average $\tilde{\omega}_{low}$ and $\tilde{\omega}_{high}$

-separate high and low frequency contributions λ_{low}, λ_{high}

$\lambda_{low} < \lambda_{high}$

ELECTRON BANDS





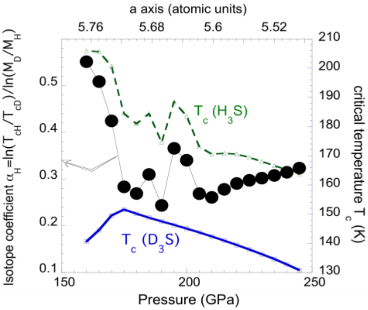
Duan, Bianconi

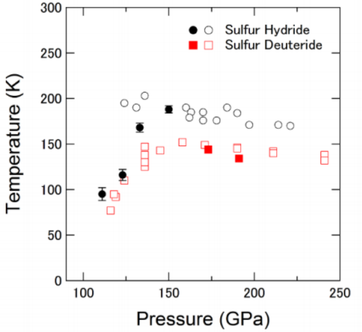
Hole pockets form in Im-3m phase with pressure

Gorkov

T_c decrease for $P > 150 GPa$ due to hole pocket coupling to high frequency phonons??

ANOMALOUS ISOTOPE EFFECT





Bianconi, Einaga

Gorkov

Possibly explained by $\lambda_{low} \approx \lambda_{high}$ in R3m phase and $\lambda_{low} < \lambda_{high}$

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END

QUESTIONS???