Superconductivity in quasiperiodic Bi-III and in YFe_2Ge_2

F. M. Grosche
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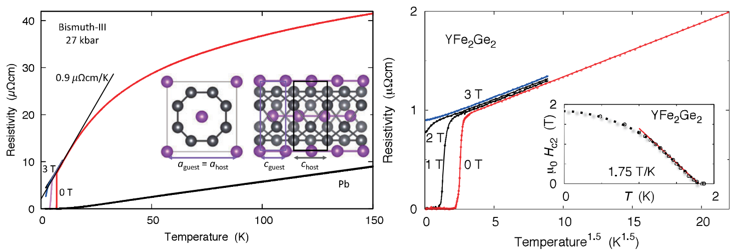


- Bi-III: incommensurate high pressure structure.
- YFe_2Ge_2: Iron-based superconductor with high $C/T \simeq 100$ mJ/molK^2.

P. Brown Sci. Adv. **4**:eaao4793 (2018). Y. Zou Phys. Status Solidi (RRL) **8,** 928 (2014)
J. Chen PRL **116,** 127001 (2016), PRB **99,** 020501(R) (2019)

Key contributors

Bi-III

- *Measurements:* **Phil Brown,** Konstantin Semeniuk
- DFT calculations: **Bartomeu Monserrat,** Chris Pickard, Diandian Wang

YFe_2Ge_2

Early work (2009-2015):
Zhuo Feng, Yang Zou, Peter Logg, Konstantin Semeniuk, Phil Brown

Next generation high purity polycrystals and single crystals:

- *Samples and characterisation:* **Jiasheng Chen** + James Tarrant
- *Quantum oscillations:* **Jordan Baglo** + Keiron Murphy
- *Heat capacity:* **Jacintha Banda** + Manuel Brando (MPI-CPfS)
- *muSR:* **Pabitra Biswas** + Adroja Devashibhai (ISIS)

Fermi surface of pressure-metallised NiS_2

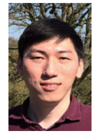
- *Crystals:* **Sven Friedema**
- *High p quantum oscillati* mann,
  meniuk, Jordan Baglo
- *High field measurements* oniglio,
  Stan Tozer (Tallahassee), Inge Leermakers, Alix McCollam (Nijmegen)

Probably won't get this far...

DFT calculations: Pascal Reiss
High pressure training and support: Patricia Alireza
Discussions with Gil Lonzarich, Christoph Geibel, Jörg Schmalian


Phil Brown


Konstantin Semeniuk

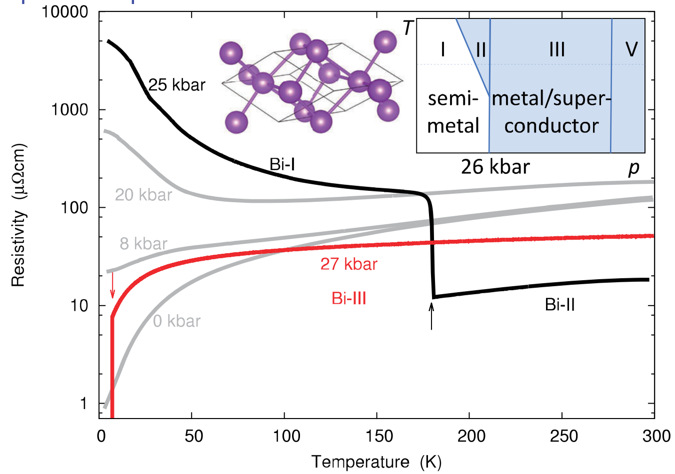

Jiasheng Chen


Jordan Baglo


Keiron Murphy


Patricia Alireza

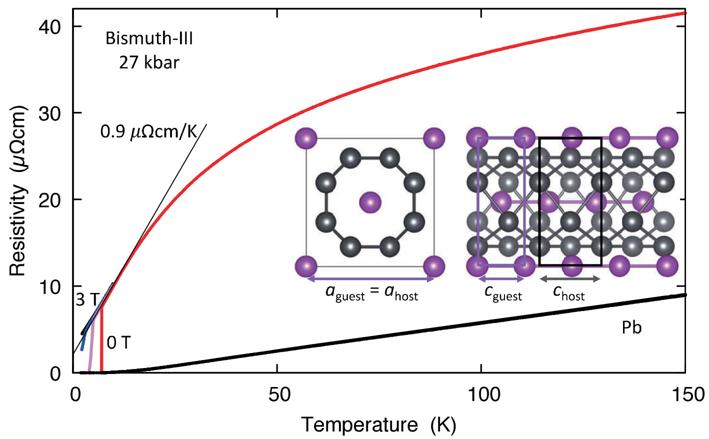
High pressure phases of Bismuth



- Semimetal with ~ 1 e$^-$ per 10^5 atoms at low pressure.
- Carrier concentration drops with increasing pressure.
- Bi-II, III: high carrier concentration, superconductivity.

P. Brown Physics Procedia **75,** 29 (2015), Li PRB **95,** 024510 (2017)

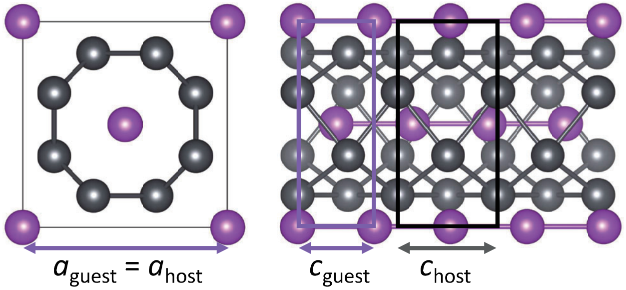
Superconductivity and T-linear resistivity in high pressure Bi-III

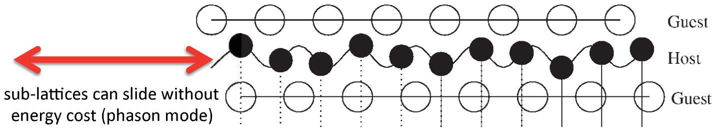


- $T_c \simeq 7.2$ K, linear $\rho(T)$ at low T.
- Compare to Pb, neighbour in periodic table, $T_c \simeq 7.2$ K.
- Incommensurate host-guest structure of Bi-III.

P. Brown Sci. Adv. **4**:eaao4793 (2018)

Bi-III phase: host-guest structure

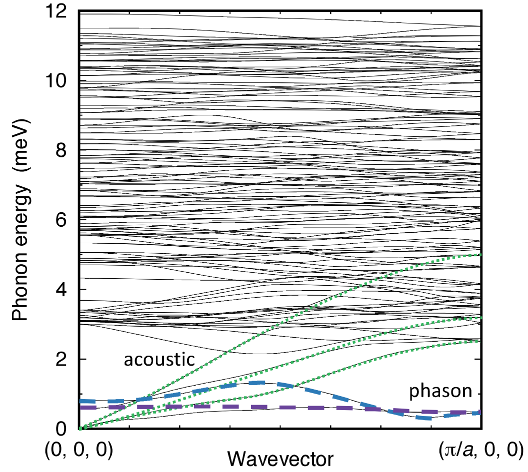




- Phason is like fourth acoustic mode (but damped).

McMahon, Degtyareva, Nelmes PRL **85**, 4896 (2000), Reed and Ackland, PRL **84**, 5580 (2000)

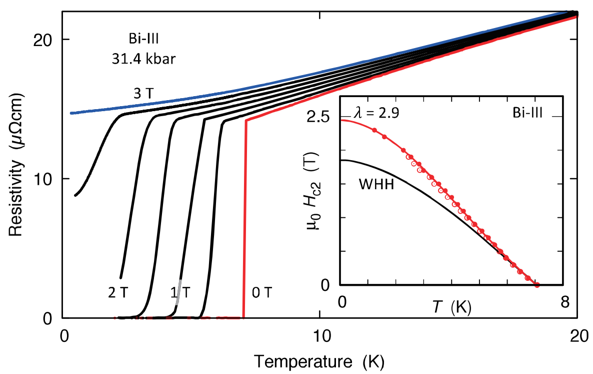
Bi-III phason modes weakly dispersive and soft



- Low-lying phason modes (2 chains per unit cell) in 42-atom mimimant
- Little dispersion perpendicular to c-axis.
- 1D dispersion $\rightarrow$ large contribution to e^--phonon λ.

Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

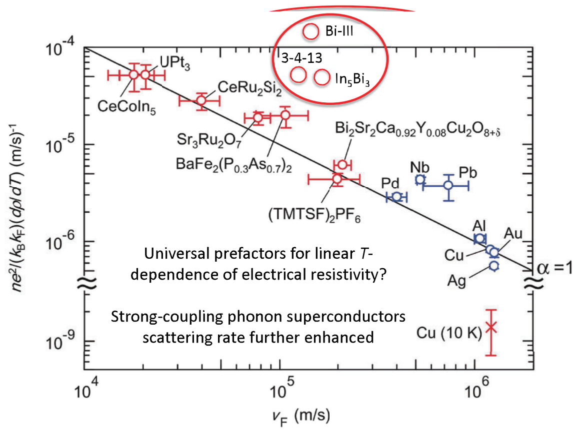
Enhanced electron-phonon coupling in high pressure Bi-III



- Scattering from low energy phonons: $\rho \propto T\lambda/\Omega_p^2$ (Ω_p = plasma freq.)
- Slope ρ' and calculated Ω_p give $\lambda \sim 2.8$. Similar λ from H_{c2} fit.
- Strong coupling, type II superconductor.
- Mass enhancement $\propto (1 + \lambda)$ explains short coherence length $\simeq$ 116 Å.

Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

Universal prefactors for linear $\rho(T)$

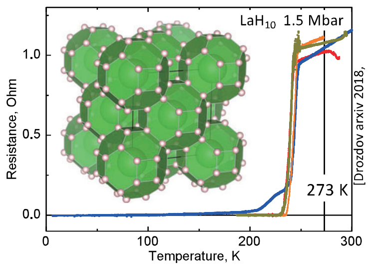


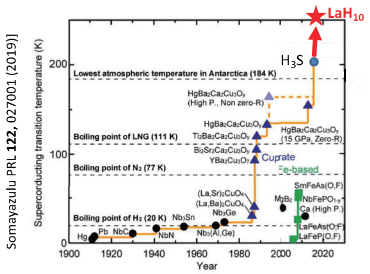
- Observation: $\hbar\tau^{-1} \sim k_B T$ (corresponds to $\alpha \simeq 1$).
- Bi-III and other strong coupling s/c: $\alpha \simeq 2\pi\lambda$.

J. Bruin, H. Sakai, R. S. Perry, A. P. Mackenzie, Science **339**, 804 (2013)

Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

Record T_c in high-pressure LaH_{10}

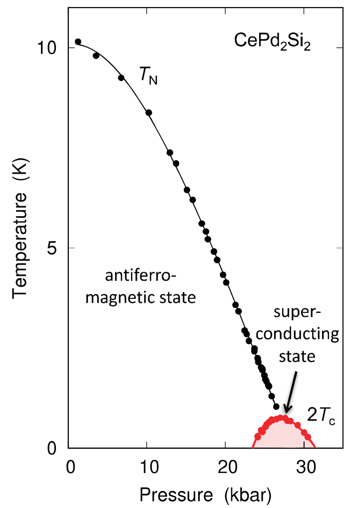


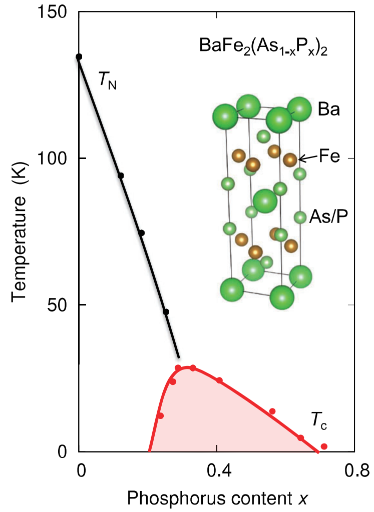


Multiple measurements by two groups, T_c extends up to 283 K: room temperature superconductivity within reach.

- Success of computationally assisted materials discovery.
- Can LaH_{10}-style superconductivity extend to ambient pressure?
- Probably not; such high phonon frequencies require compression.
- Need alternative pairing interaction with high energy scale: **magnetic interaction in metals reaches up to 3,000 K.**

From narrow-band, f-electron low-T_c to d-electron high-T_c

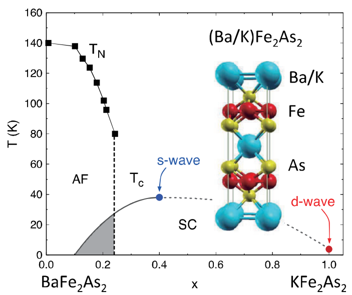


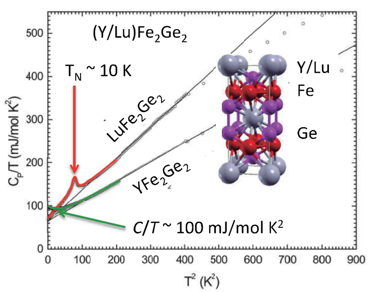


We need more unconventional superconductors!

Mathur Nature **394**, 39 (1998), Hashimoto Science **336**, 1554 (2012)

From KFe_2As_2 to YFe_2Ge_2

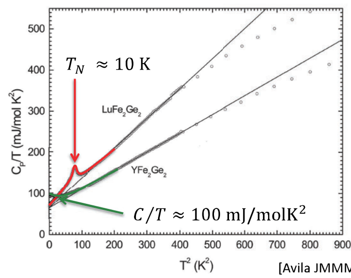


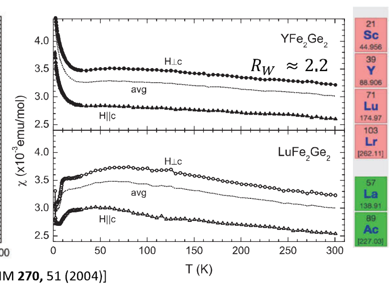


- Search for analogues to Fe-As superconductors.
- KFe_2As_2 ($T_c \simeq 3.8$ K): high $C/T \simeq 100$ mJ/mol K^2.
- YFe_2Ge_2 has similarly high C/T, apparently same Fe oxidation number as in KFe_2As_2.

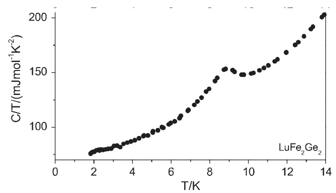
Reid Supercond. Sci. Technol. **25,** 084013 (2012), Avila JMMM **270,** 51 (2004)

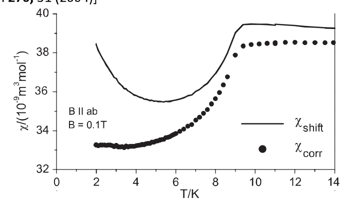
Early work on (Y/Lu)Fe_2Ge_2





[Avila JMMM **270**, 51 (2004)]



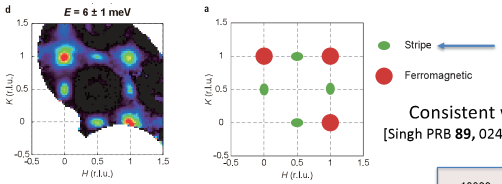


[Ferstl Physica B **378–380**, 744 (2006)]

- Antiferromagnetic transition in $LuFe_2Ge_2$ near 10 K.
- Magnetic susceptibility $\chi_{SI} \sim 10^{-3}$. Moderately enhanced Wilson ratio $R_W \simeq 2.5$.

Neutron scattering in YFe_2Ge_2

[Wo Phys. Rev. Lett. **122**, 217003 (2019)]

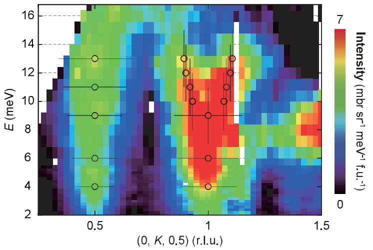


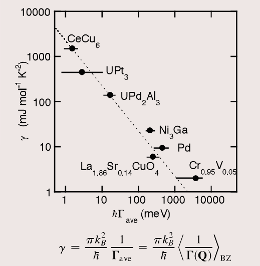
as in FeAs

FM planes, stacked afm

Consistent with early DFT studies

[Singh PRB **89**, 024505 (2014), Subedi ibid 024504]



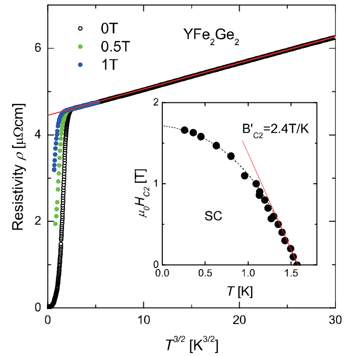


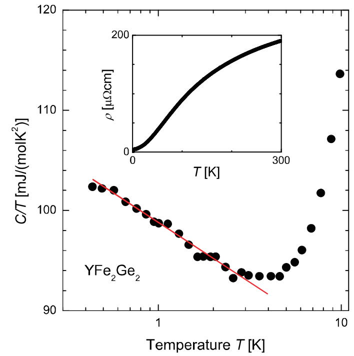
$$\gamma = \frac{\pi k_B^2}{\hbar}\frac{1}{\Gamma_{ave}} = \frac{\pi k_B^2}{\hbar}\left\langle \frac{1}{\Gamma(\mathbf{Q})} \right\rangle_{BZ}$$

[Hayden PRL **84**, 999 (2000)]

Data show fluctuations at two Q-vectors, but appear not sufficient to explain high γ.

Superconductivity in YFe_2Ge_2, first-generation samples



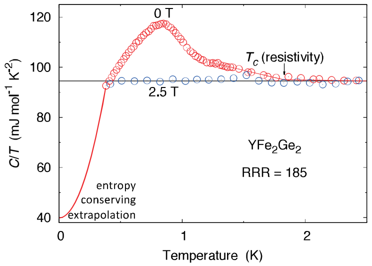


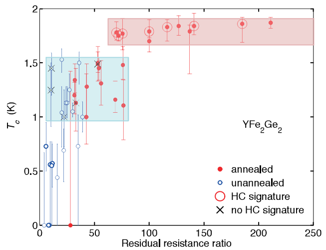
- Polycrystals (induction-furnace) or single crystals (flux).
- Resistance ratios < 60.
- Resistive transitions but no heat capacity anomaly at T_c.

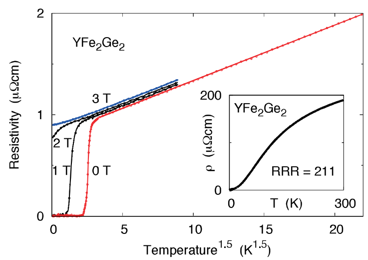
[Zou Phys Status Solidi (RRL) **8**, 928 (2014); Kim Phil. Mag. **95**, 804 (2015)]

Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

Growth improvements lead to bulk superconductivity in polycrystals





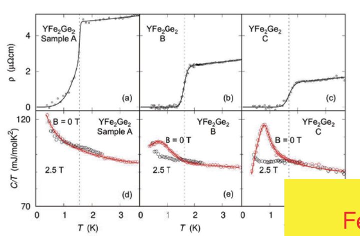


- Induction furnace. Pre-reaction. Anneal 1h at 1250 °C, 1 week at 800 °C.
- RRR > 70: sharp resistive transitions and superconducting heat capacity anomalies.
- Residual $\gamma \sim 40$ mJ/molK^2.
- Anomalous normal state: $\rho = \rho_0 + AT^{3/2}$
- B_{c2} suggests $\xi \approx 120$ Å.

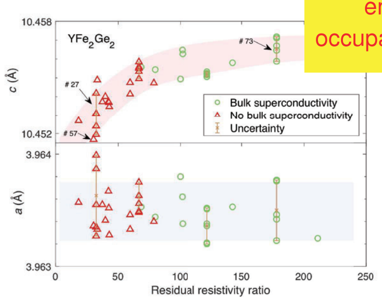
[Chen PRL **116**, 127001 (2016)]

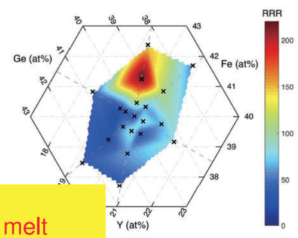
Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

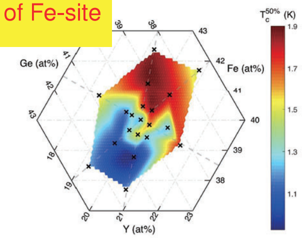
Growth study in YFe_2Ge_2 polycrystals



Fe-rich melt ensures full occupation of Fe-site





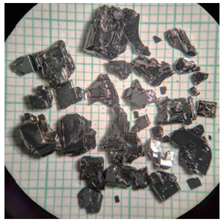


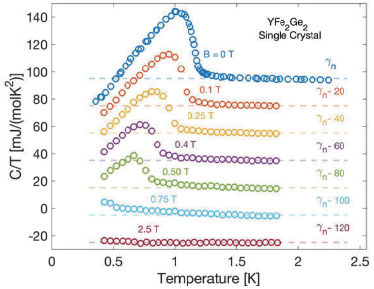
[Chen et al, PRB **99**, 020501(R) (2019)]

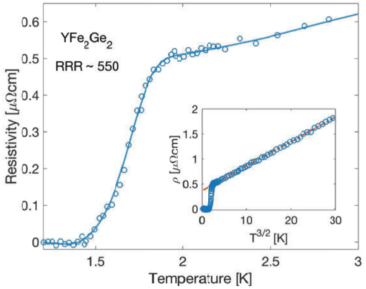
Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

Towards high quality single crystals of YFe_2Ge_2

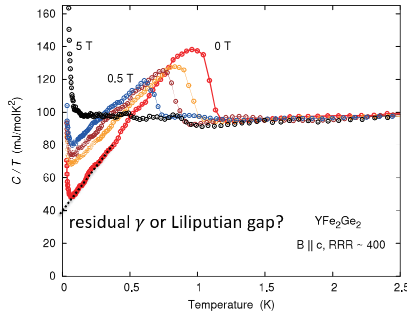
- Sn flux growth from high quality polycrystals (grown from Fe-rich melt).
- Experimenting with temperature profiles, crucible orientation, growth protocol has gradually produced **RRR ~ 500.**
- Sharp bulk transitions. Resistivity still $T^{3/2}$.



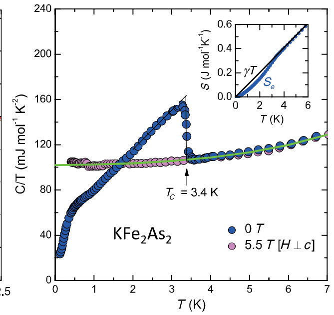




Heat capacity to very low temperatures



[J. Banda MPI-CPfS, data just in]

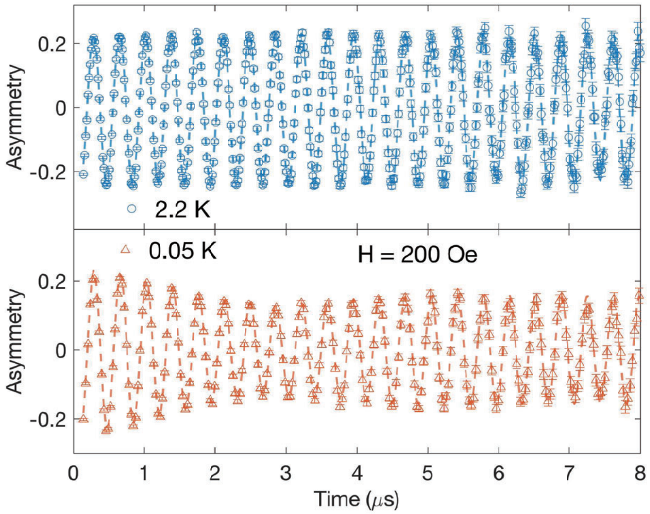


[Hardy PRL **111**, 027002 (2013)]

- Dilution fridge measurements confirm sharp bulk transition in new generation of YFe_2Ge_2 single crystals.
- Upturn at low temperature (nuclear contribution) prevents definitive conclusion about gap structure and residual γ.
- Similarity with KFe_2As_2.

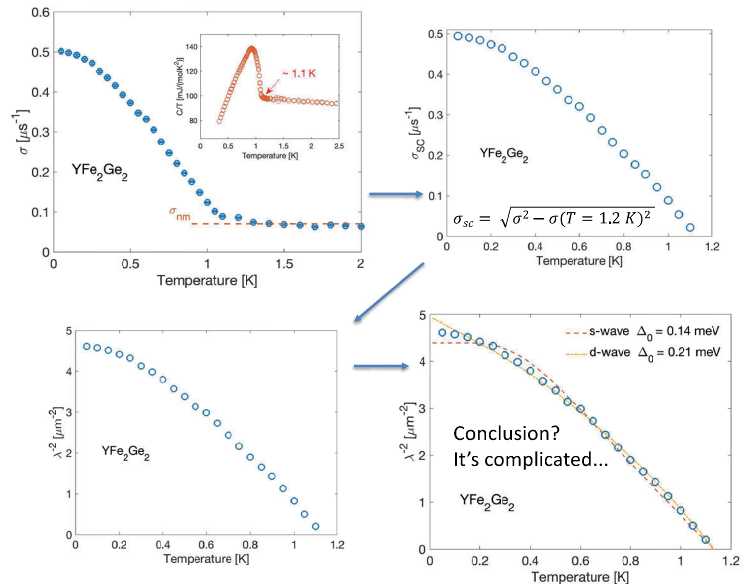
Transverse field muSR measurements

$$A_{TF} = A_0 \exp(-(\sigma t)^2/2)\cos(\gamma\mu\langle B\rangle t + \phi) + A_{bg}\cos(\gamma\mu B_{bg} t + \phi)$$

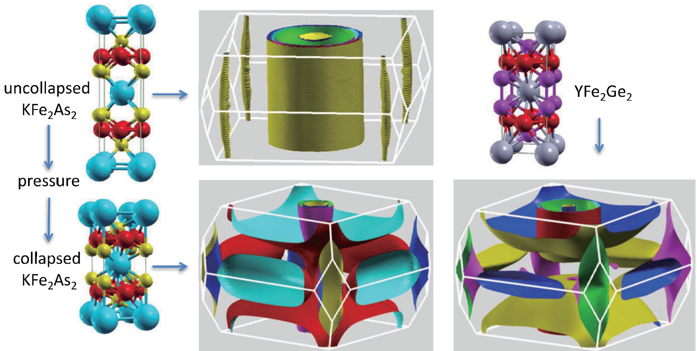


First attempt at ISIS with Pabitra Biswas and Adroja Devashibhai

Transverse field muSR



High pressure KFe_2As_2 similar to YFe_2Ge_2

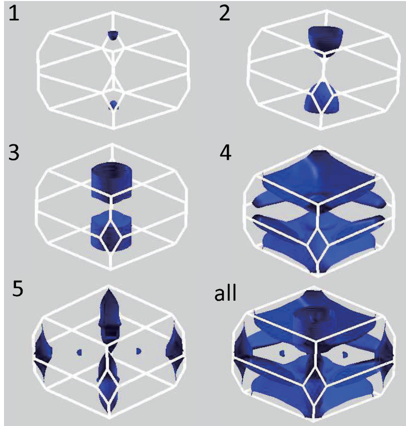


YFe_2Ge_2 Fermi surface resembles that of KFe_2As_2 in **collapsed tetragonal** phase.

RFe_2X_2	c/a	X-X dist. (Å)
uct KFe_2As_2 ($p = 0$)	3.608	4.089
ct KFe_2As_2 (21 GPa)	2.491	2.544
YFe_2Ge_2	2.639	2.721

Ge-Ge or As-As bond: Fe $d^{5.5} \to d^{6.5}$

YFe_2Ge_2 calculated Fermi surface sheets



Sheet	Freq. (kT)	Mass (m_e)
2 (B||a)	4.25	2.49
3 (B||a)	5.86	2.71
4 (B||a)	11.90	2.86
5 (B||c)	0.95	1.67

(our Wien2k calc.)

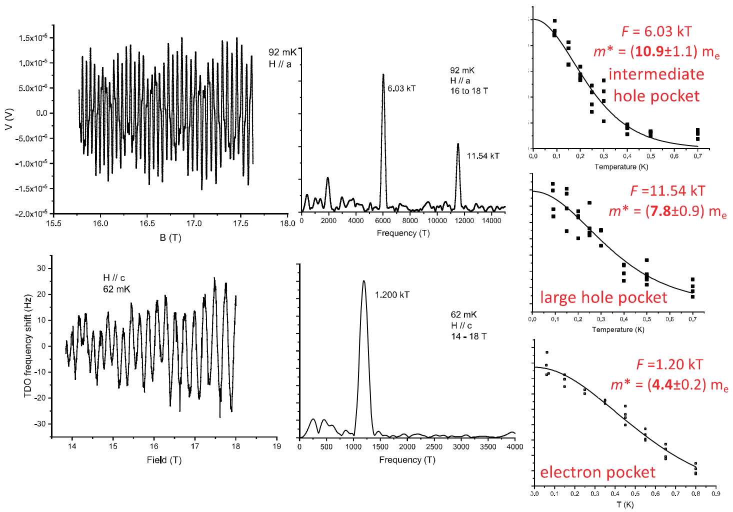
DFT predicts $\gamma \simeq 16$ mJ/molK^2 vs. measured 100 mJ/molK^2.

Expect measured masses of order 10 m_e.

[Singh PRB **89**, 024505, Subedi PRB **89**, 024504 (2014)]

Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

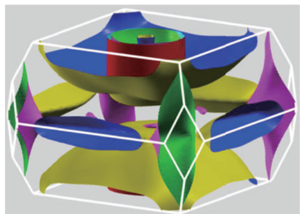
May 2019 quantum oscillation data



Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
New superconductors
The route to YFe_2Ge_2
KFe_2As_2 / YFe_2Ge_2
The (Lu/Y)Fe_2Ge_2 system
Neutrons
First-generation samples
Growth studies
High purity YFe_2Ge_2
Heat capacity
muSR
Fermi surface structure
YFG Summary
Summary

Summary YFe_2Ge_2

Sheet	Freq. (kT)	Mass (m_e)	Freq. (kT)	Mass (m_e)	m_{exp}/m_{DFT}
	DFT		experiment		
2 (B||a)	4.25	2.49	n/a	n/a	
3 (B||a)	5.86	2.71	6.03	10.9	4
4 (B||a)	11.90	2.86	11.54	7.8	2.7
5 (B||c)	0.95	1.67	1.20	4.4	2.6



- Origin of high heat capacity?
- Superconductivity: residual γ or tiny second gap? Nodes?
- Origin of anomalous $T^{3/2}$ normal state resistivity?
- **Bulk properties as in KFe_2As_2 – but different Fermi surface.**

Superconductivity in Bi-III and YFe_2Ge_2
QSC 24/6/2019
Introduction
Host-guest structures
Bismuth under pressure
Bi-III
Lattice and phonons
Sliding mode
Phonon dispersion
Strong coupling superconductivity
Linear resistivity
YFe_2Ge_2
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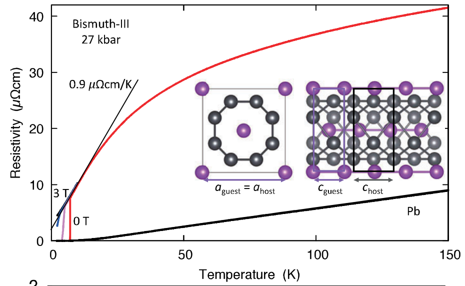
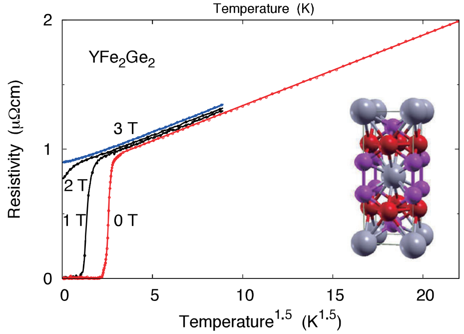
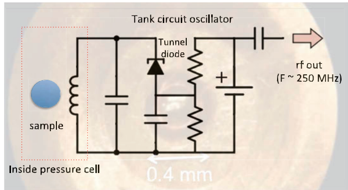
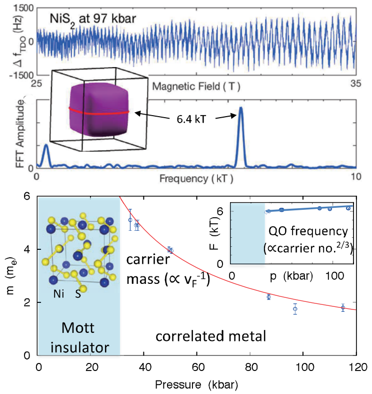

Bismuth-III
27 kbar
0.9 μΩcm/K
Resistivity (μΩcm)
3 T
0 T
Pb
Temperature (K)


YFe2Ge2
Resistivity (μΩcm)
3 T
2 T
1 T
0 T
Temperature1.5 (K1.5)


Tank circuit oscillator
Tunnel diode
rf out
(F ~ 250 MHz)
sample
Inside pressure cell
0.4 mm


NiS2 at 97 kbar
Magnetic Field (T)
FFT Amplitude
6.4 kT
Frequency (kT)
carrier
mass (∝ vF-1)
QO frequency
(∝carrier no.2/3)
p (kbar)
Ni S
Mott
insulator
correlated metal
Pressure (kbar)