High pressure studies on magnetism and lattice dynamics by Nuclear Resonance Scattering

Ilya Sergeev, DESY, Hamburg

Outline

- High pressure studies with Nuclear Forward Scattering:
  Search for the collapse of magnetism in Ni.

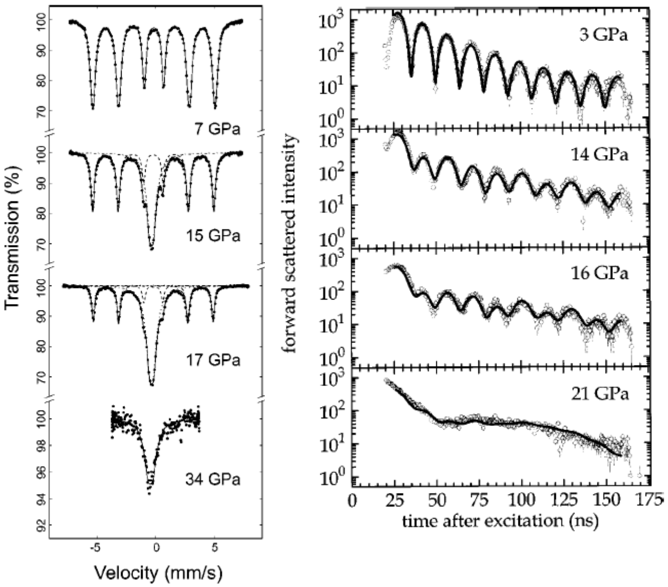
- High pressure studies with Nuclear Inelastic Scattering:
  Search for the non-magnetic state of Fe-superconductors

NFS studies at high pressure

Interactions 123/124 (1999) 529–559

High-pressure studies with nuclear scattering of synchrotron radiation

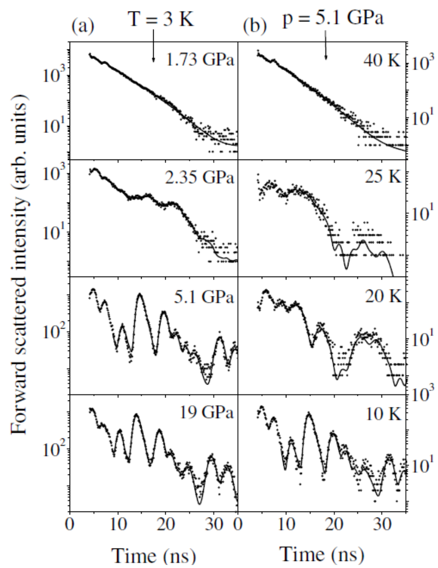
Rainer Lübbers [a], Gerhard Wortmann [a] and Hermann F. Grünsteudel [b]

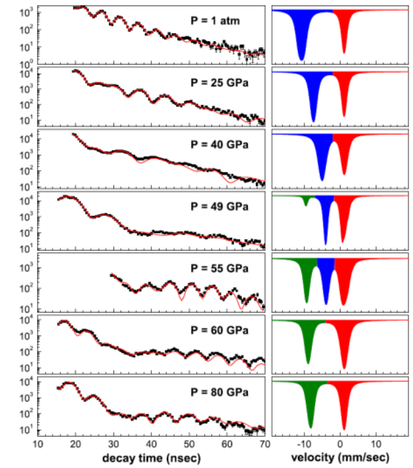


PRL 109, 026403 (2012) PHYSICAL REVIEW LETTERS week ending 13 JULY 2012

Reentrant Valence Transition in EuO at High Pressures: Beyond the Bond-Valence Model

N. M. Souza-Neto,[1,2,*] J. Zhao,[1] E. E. Alp,[1] G. Shen,[3] S. V. Sinogeikin,[3] G. Lapertot,[4] and D. Haskel[1,†]





VOLUME 92, NUMBER 6 PHYSICAL REVIEW LETTERS week ending 13 FEBRUARY 2004

Pressure-Induced Magnetic Order in Golden SmS

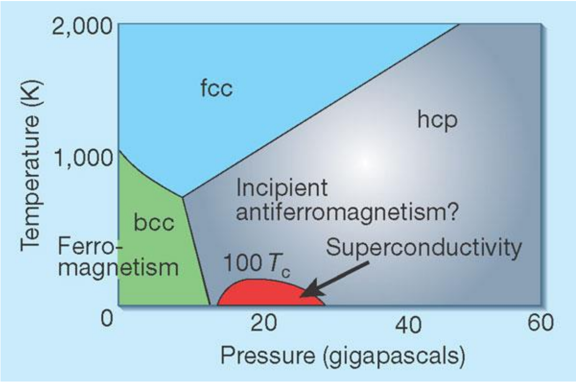
A. Barla,[1] J. P. Sanchez,[2] Y. Haga,[2,3] G. Lapertot,[2] B. P. Doyle,[1,*] O. Leupold,[1] R. Rüffer,[1] M. M. Abd-Elmeguid,[4] R. Lengsdorf,[4] and J. Flouquet[2]

- Main goal: study of magnetic and electronic properties (e.g. valence change) under compression
- Can be applied to different Mossbauer isotopes: ^{57}Fe, ^{119}Sn, ^{151}Eu, ^{149}Sm, ^{125}Te, ^{121}Sb, ^{61}Ni

Magnetism in 3d metals at compression

Fe:

magnetic α(bcc) →
non-magnetic ε(hcp) at ~**16 GPa**
Collapse of magnetism
due to the phase transition



Ni:

Ni has stable structures under compression

- **Ni:** fcc phase up to at least 200 GPa

At ambient conditions

- **Ni:** ferromagnetic with Tc = 630K

Ni is a good candidates to investigate evolution of magnetic moment with high compression.

^{61}Ni is the Mossbauer isotope with nuclear transition energy – 67 keV

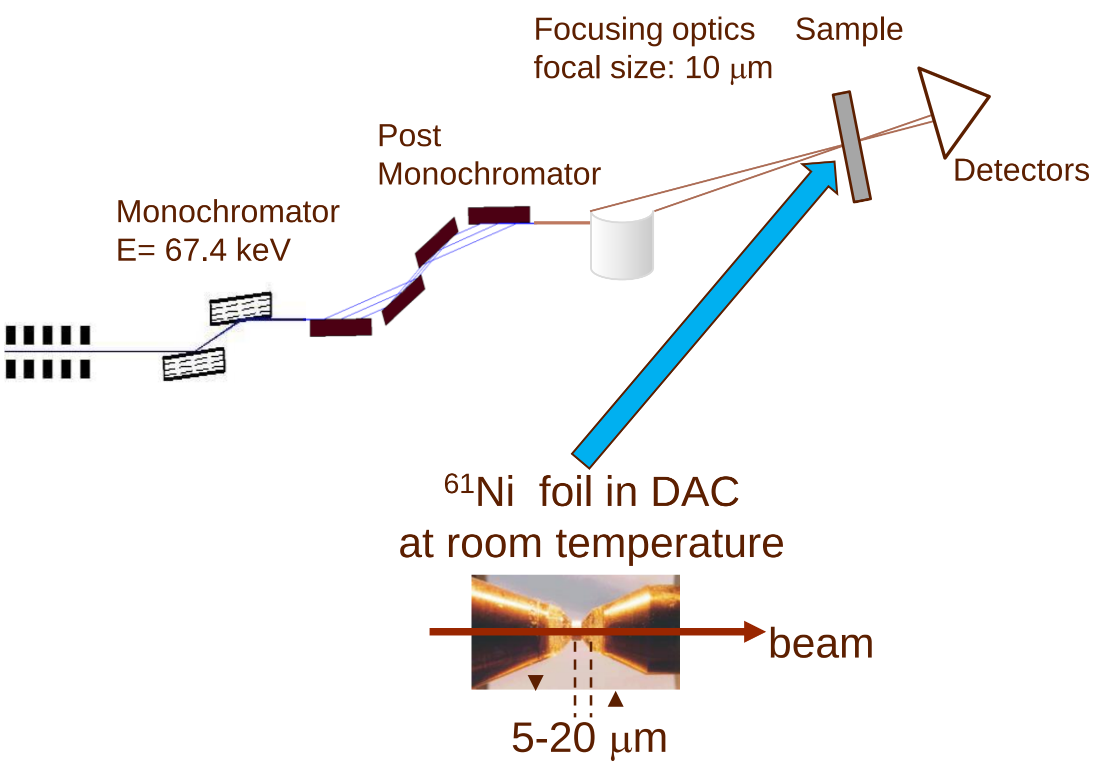
Highest pressure for magnetism

PRL **111,** 157601 (2013) PHYSICAL REVIEW LETTERS week ending 11 OCTOBER 2013

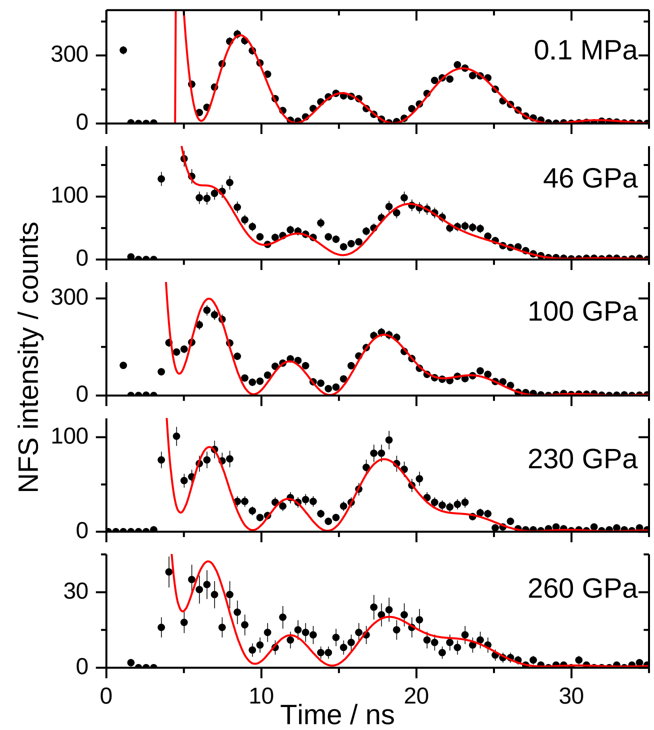
Hyperfine Splitting and Room-Temperature Ferromagnetism of Ni at Multimegabar Pressure

I. Sergueev,[1,*] L. Dubrovinsky,[2] M. Ekholm,[3] O. Yu. Vekilova,[4] A. I. Chumakov,[5] M. Zając,[5] V. Potapkin,[5,2] I. Kantor,[5] S. Bornemann,[6] H. Ebert,[6] S. I. Simak,[4] I. A. Abrikosov,[4] and R. Rüffer[5]

Experimental setup



Measurements

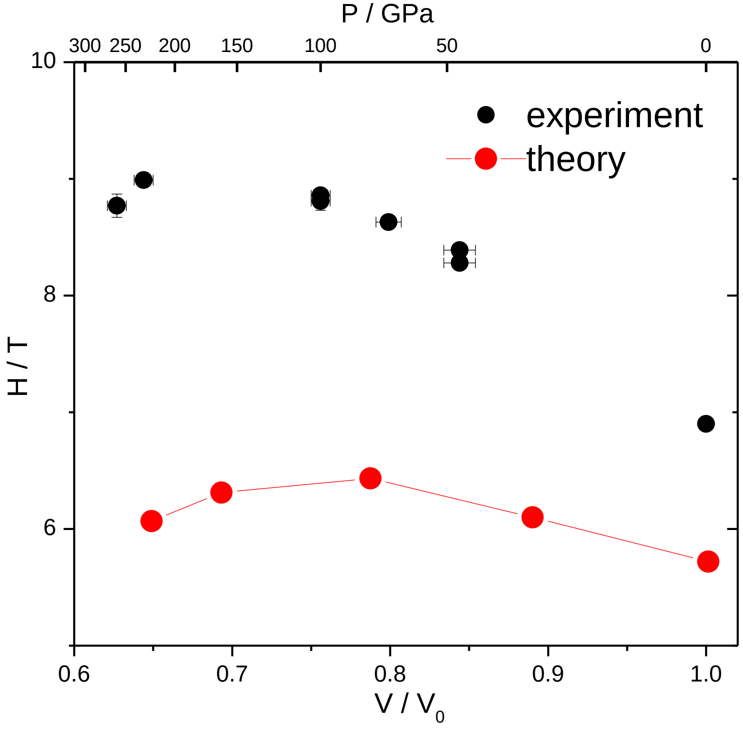


$$I(t) \sim \sum A_i \cos(f_i \cdot H \cdot t)$$

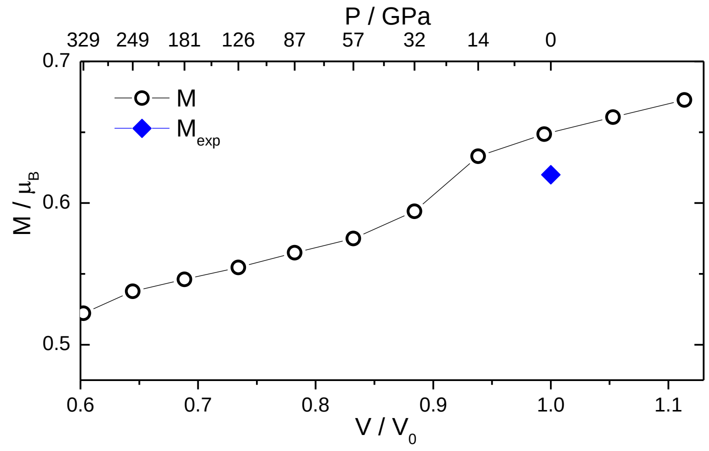
H – hyperfine magnetic field

Highest pressure for magnetism

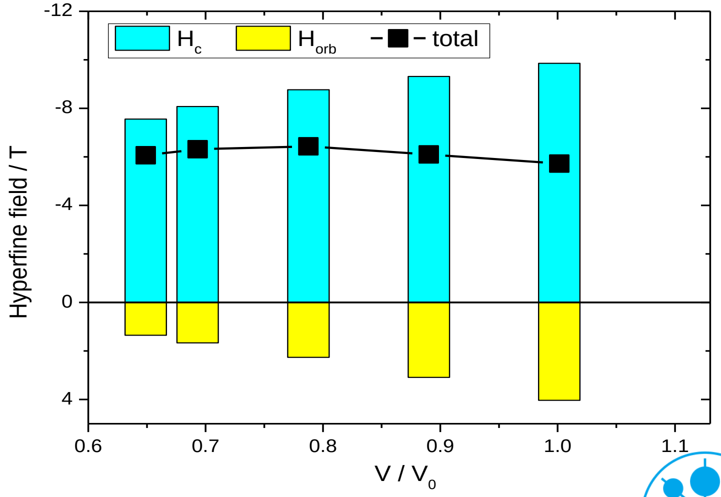
Experiment and theory



Magnetic moment vs volume (theory)



Hyp. magn. field vs volume (theory)

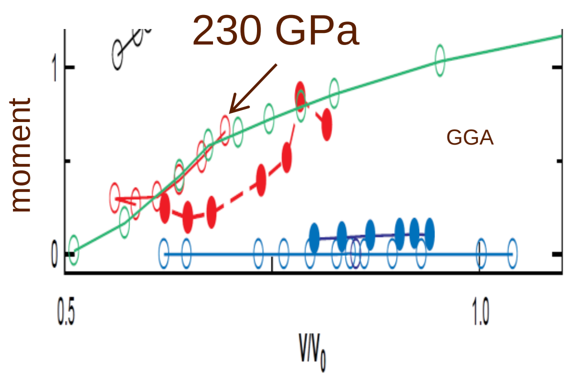


- Ni is ferromagnetic at room temperature up to 260 GPa.
- Measurements at higher pressure are required in order to find critical pressure.

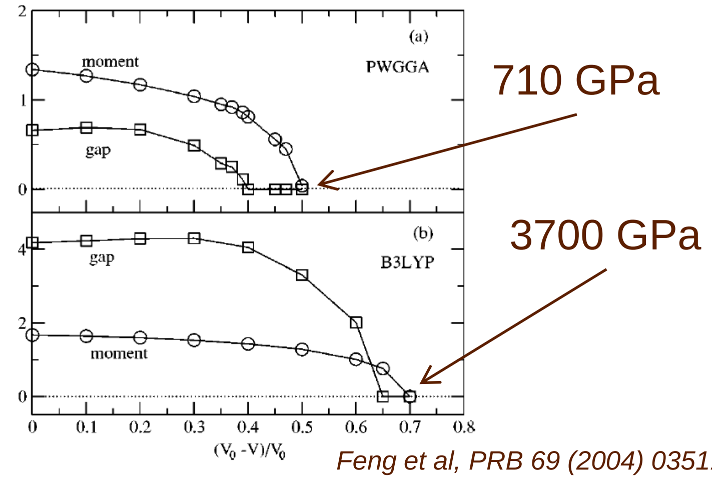
NiO at High Pressure

NiO – antiferromagnetic insulator at 0GPa.
The magnetic collapse and metal-insulator transitions are expected at high pressure

Theory:



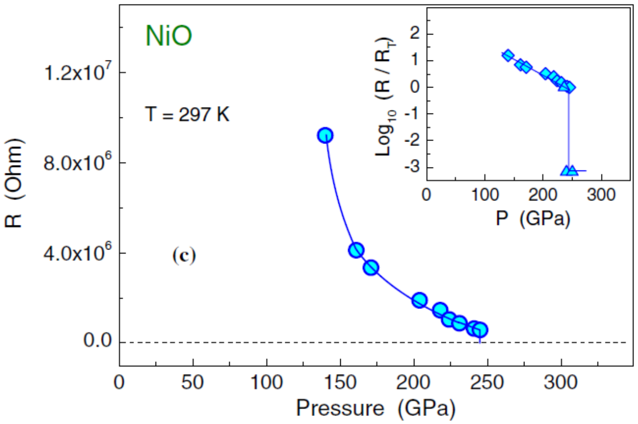
Cohen et al, Science 275 (1997) 654



Feng et al, PRB 69 (2004) 035114

Experiment:

Transition to metallic state at 240GPa is reported



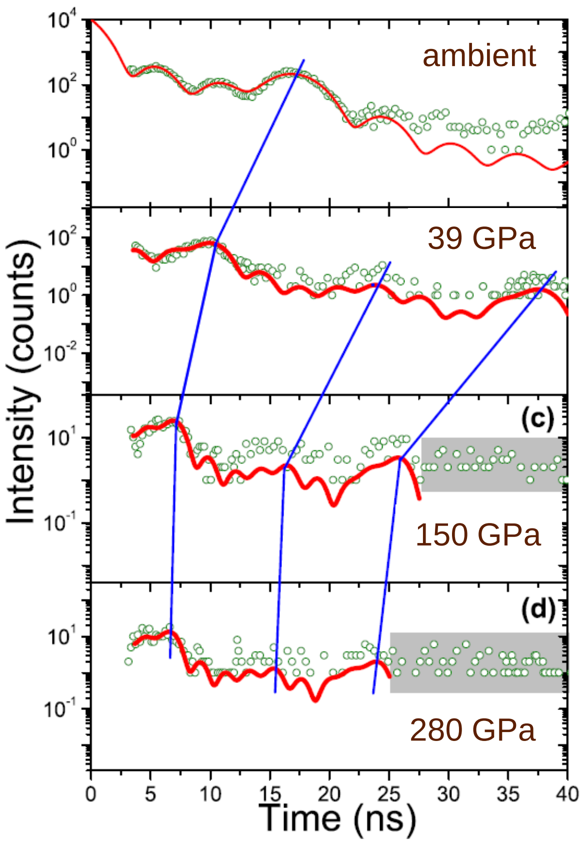
Gavriliuk et al,
PRL 109 (2012) 086402

NFS measurements with NiO at high pressures

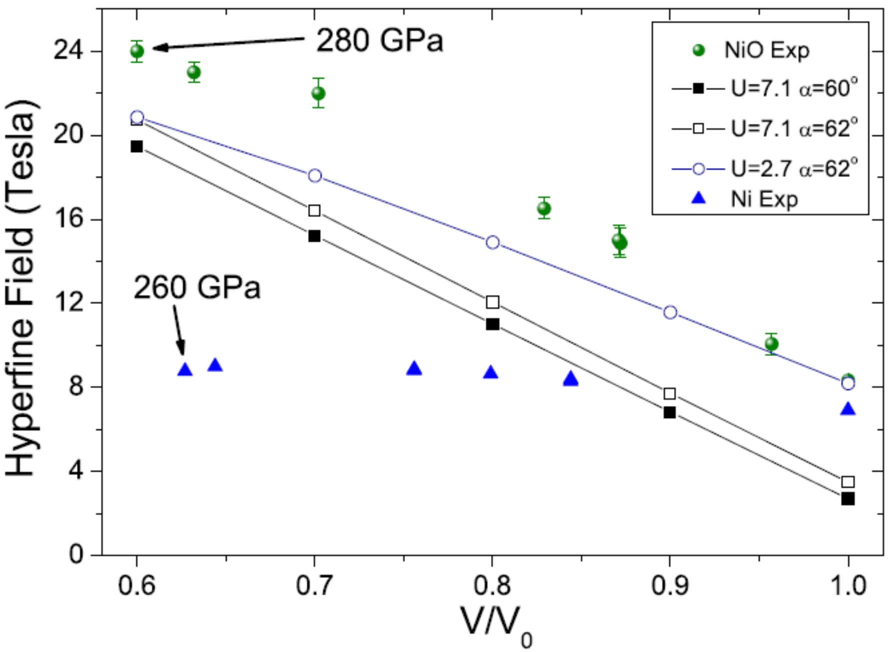
PHYSICAL REVIEW B 93, 201110(R) (2016)

Magnetic interactions in NiO at ultrahigh pressure

V. Potapkin,[1,*] L. Dubrovinsky,[2] I. Sergueev,[3] M. Ekholm,[4] I. Kantor,[5] D. Bessas,[5] E. Bykova,[2] V. Prakapenka,[6] R. P. Hermann,[1,7] R. Rüffer,[5] V. Cerantola,[2] H. J. M. Jönsson,[8] W. Olovsson,[8] S. Mankovsky,[9] H. Ebert,[9] and I. A. Abrikosov[4,10,11]



Hyperfine magnetic field vs compression



Study confirms magnetic state of NiO up to 280 GPa

Looking forward on HP ^{61}Ni NFS with EBS

Search for magnetic collapse in Ni and NiO requires study at pressures above 3 Mbar

1. Energy of ^{61}Ni nuclear transition is 67 keV. Width of the transition is 100 neV.
   Flux is the most important issue for the measurements.

2. Pressures above 3 Mbar requires ds-DAC and small beam size.
   Beam size of ~1 um (with full flux) is an issue for the measurements.

EBS features:

1. Increase of the energy flux density at high energies.

2. Decrease of the source size (in horizontal direction)
   Leads immediately to the factor 2 in flux with the same optics.

Beam size issue is valid not only for ^{61}Ni but also for other isotopes (^{57}Fe, ^{119}Sn, ^{151}Sm, ^{149}Eu)

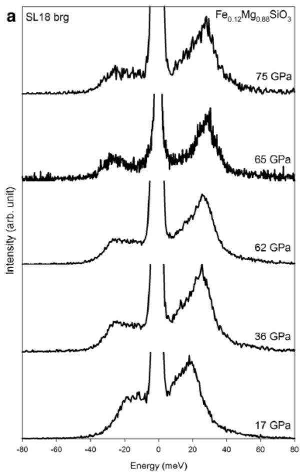
NIS studies at high pressures

McCammon *et al. Progress in Earth and Planetary Science* (2016) 3:10
DOI 10.1186/s40645-016-0089-2
Progress in Earth and Planetary Science

RESEARCH ARTICLE Open Access

Sound velocities of bridgmanite from density of states determined by nuclear inelastic scattering and first-principles calculations

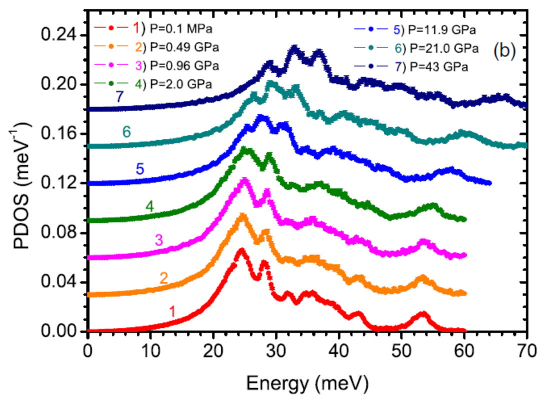
Catherine McCammon[1*], Razvan Caracas[2], Konstantin Glazyrin[3], Vasily Potapkin[1], Anastasia Kantor[1,4], Ryosuke Sinmyo[1,6], Clemens Prescher[1,7], Ilya Kupenko[1,4,8], Aleksandr Chumakov[4,5] and Leonid Dubrovinsky[1]



PHYSICAL REVIEW B **93**, 081102(R) (2016)

Experimental observation of phonons as spectators in FeSi electronic gap formation

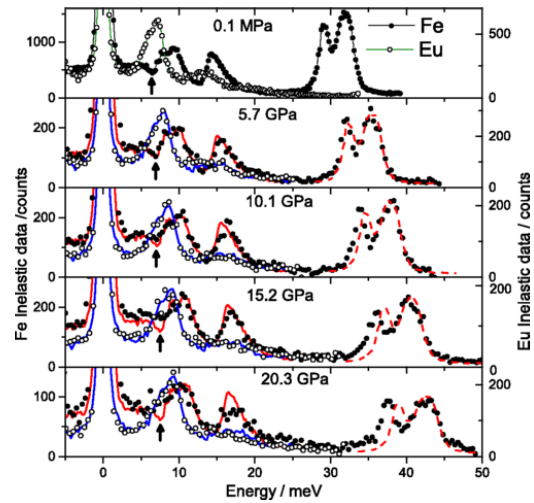
P. P. Parshin,[1,*] A. I. Chumakov,[1,2] P. A. Alekseev,[1,3] K. S. Nemkovski,[4] J. Perßon,[5] L. Dubrovinsky,[6] A. Kantor,[2,6] and R. Rüffer[2]



PHYSICAL REVIEW B **91**, 224304 (2015)

Quenching rattling modes in skutterudites with pressure

I. Sergueev,[1,*] K. Glazyrin,[1] I. Kantor,[2] M. A. McGuire,[3] A. I. Chumakov,[2] B. Klobes,[4] B. C. Sales,[3] and R. P. Hermann[3,4,5]



Possible applications:

- Elastic/thermodynamic properties (sound velocity, mean square displacement, temperature, entropy)
- Anharmonic properties (Gruneisen parameter) for thermal conductivity, thermoelectrics
- Investigation of material properties (electronic, magnetic) versus e-ph coupling.

Fe-superconductors. Overview

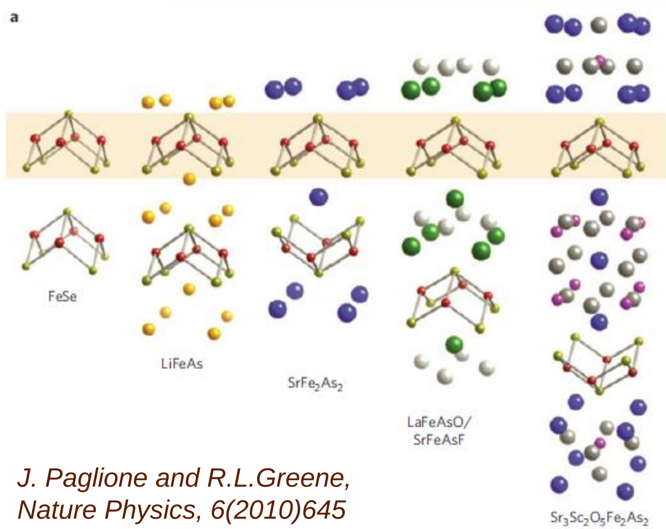
J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

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

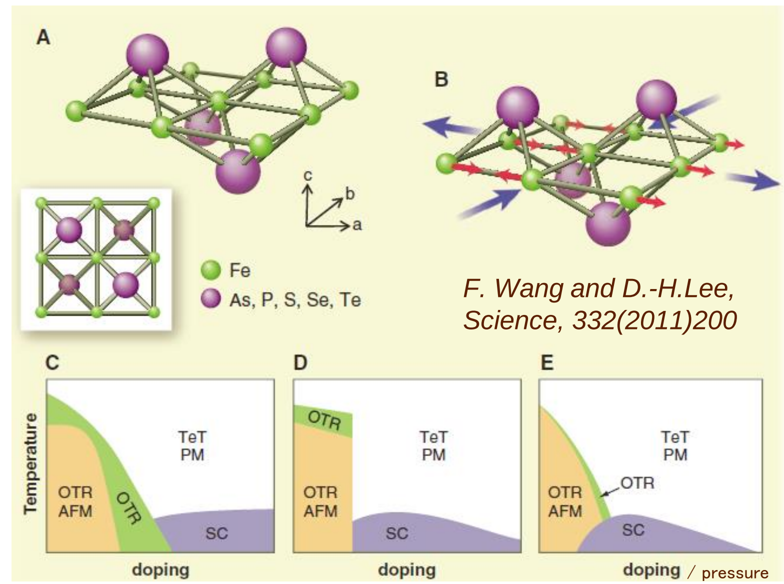
Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

Crystallographic structures of Fe-superconductors



J. Paglione and R.L.Greene, Nature Physics, 6(2010)645

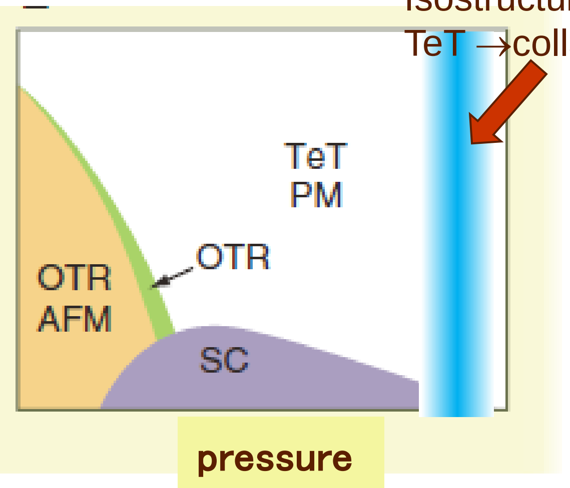
Phase diagrams of Fe-superconductors



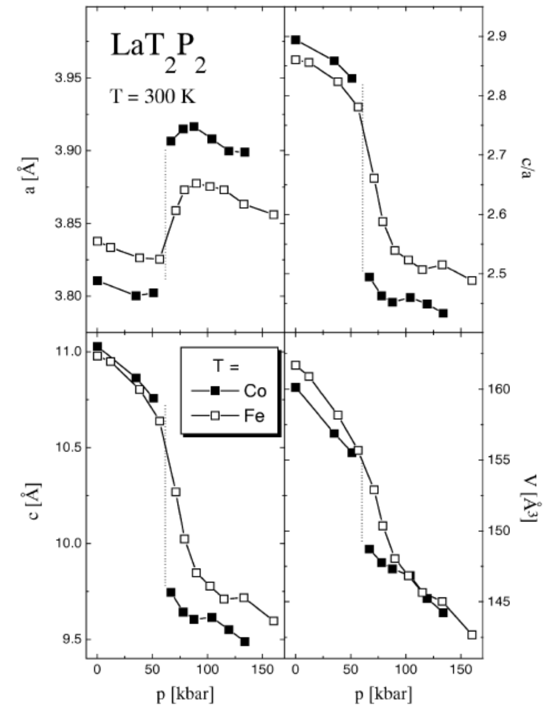
F. Wang and D.-H.Lee, Science, 332(2011)200

- superconductivity originates within Fe layer
- suppression of magnetism by doping or by pressure leads to SC
- unconventional superconductors: magnetic(?) excitations are the “glue” of the Cooper pair

Isostructural transition at 122 family

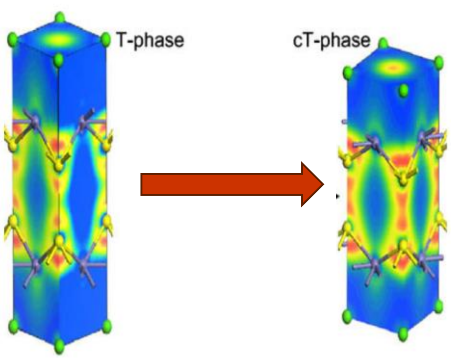


This transition is common for $ThCr_2Si_2$-type structure



C. Huhnt et al. / Physica B 252 (1998) 44

Transition is due to the formation of the As-As interlayer electronic bonds

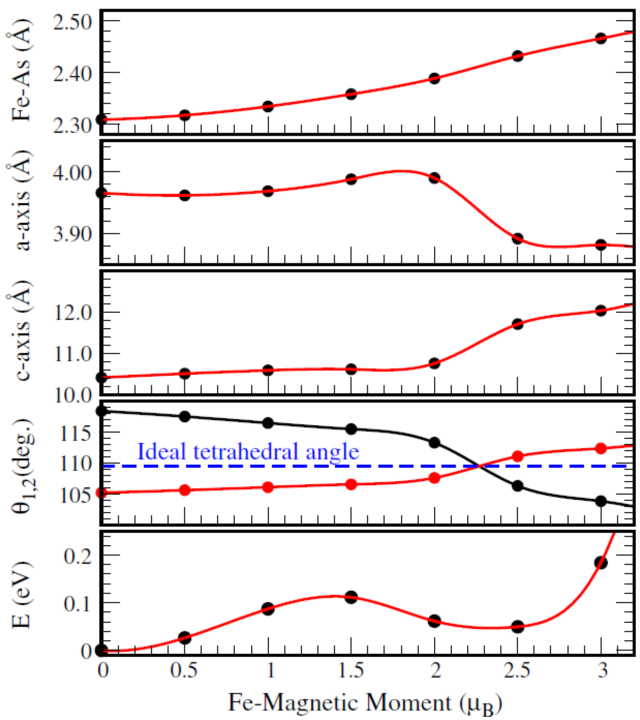


This transition - electronic topological transition where Fermi surface changes from 2D to 3D type (Lifshitz transition)

Isostructural transition and magnetism. Theory

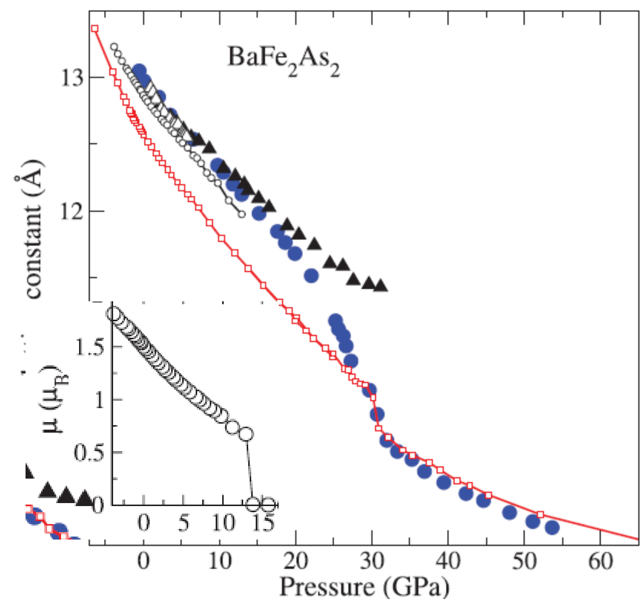
2 approaches

T. Yildirim, Phys. Rev. Lett *102 (2009) 037003*



As-As hybridization is controlled by Fe spin state. Fe magnetic moment is totally lost or strongly reduced in cT phase

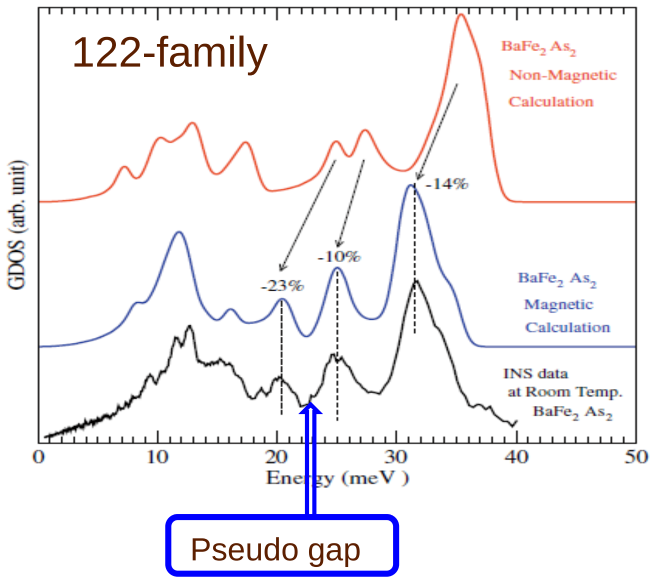
Colonna, PRB 83(2011) 094529



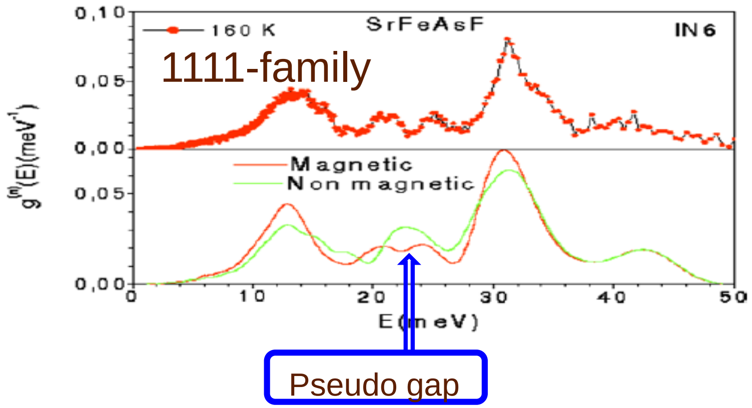
The collapse of Fe-magnetic moment is well separated from T-cT transition. The last transition is pure electronic transition and has nothing to do with Fe spin state

Theory. Coupling of phonons and magnetism

T. Yildirim, Physica C 469(2009) 425

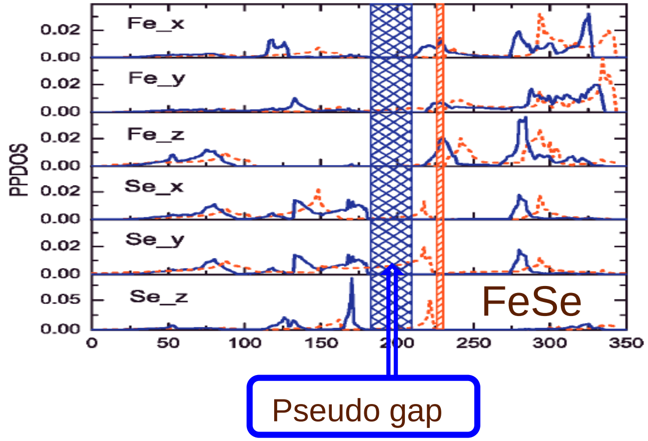


Zbiri et al.,J.Phys.Cond.Matt. 22(2010)315701



Wang et al.,Physica C 472(2012)29

11-family



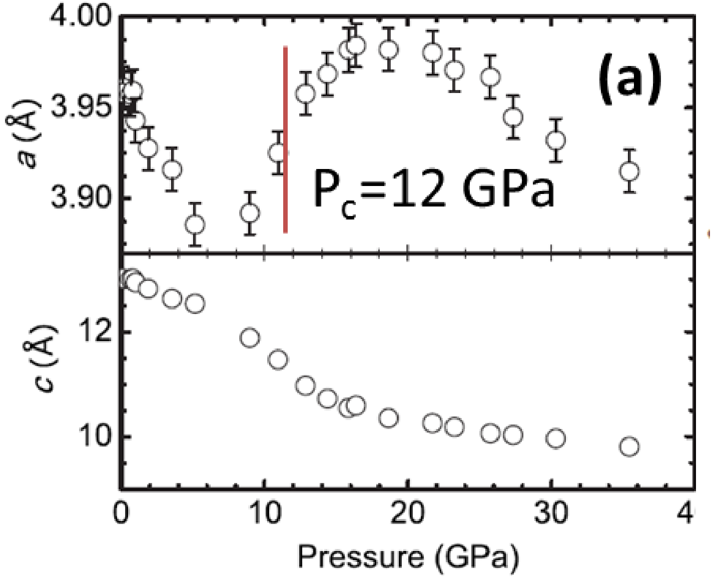
Theory predicts significant effect of the local magnetic moment on the phonon structure.

Pseudo gap at 20-26 meV is seen only with spin-polarized calculations

$BaFe_2As_2$. Pressure behaviour with XRD

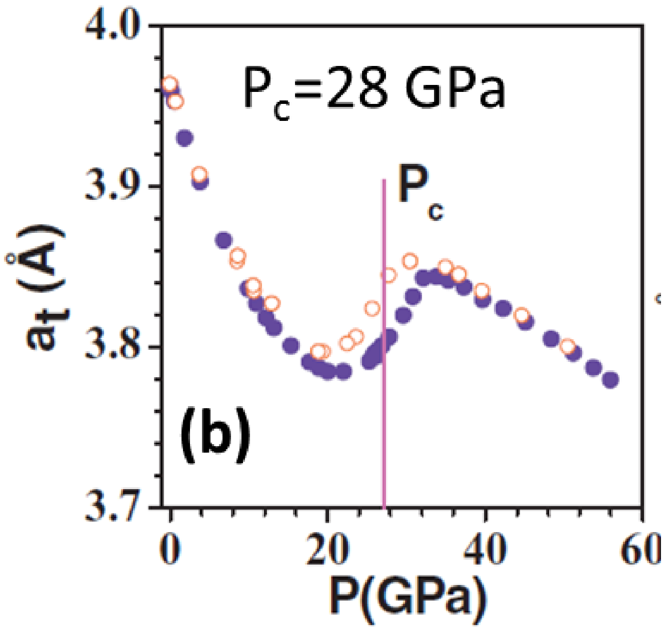
Crystal with c-axis along diamonds,
No pressure medium

Uhoya et al., PRB 82, 144118 (2010)



Polycrystal,
Ne pressure medium

Mittal et al., PRB 83, 054503 (2011)



Critical pressure of T-cT transition strongly depends on pressure conditions
(hydrostaticity, direction of applied force)

$BaFe_2As_2$. NIS study at HP

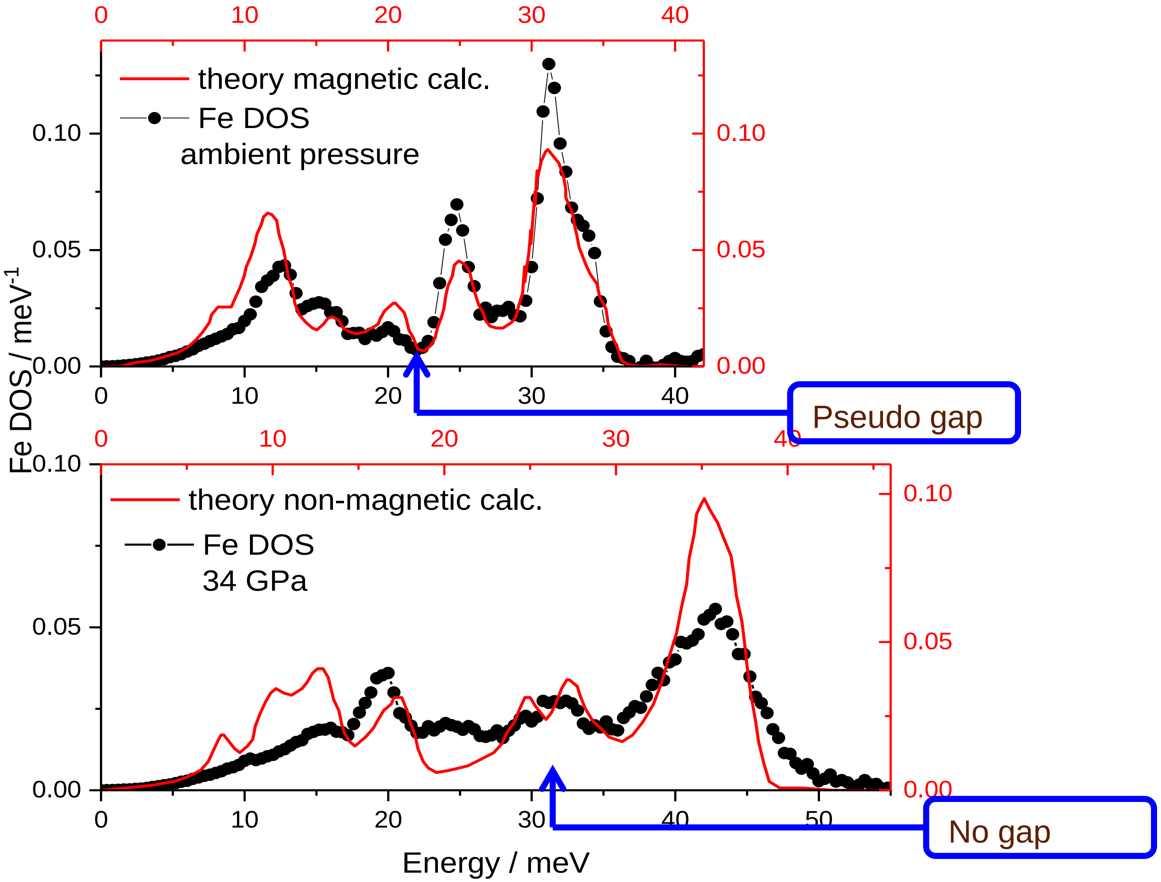
Sample:
$BaFe_2As_2$ crystal in DAC with c-axis along diamond
Pressure medium: paraffin oil

Method:
NIS using ^{57}Fe nuclear resonance

Measurements at room T.

Theory

Yildirim, Physica C 469(2009)425

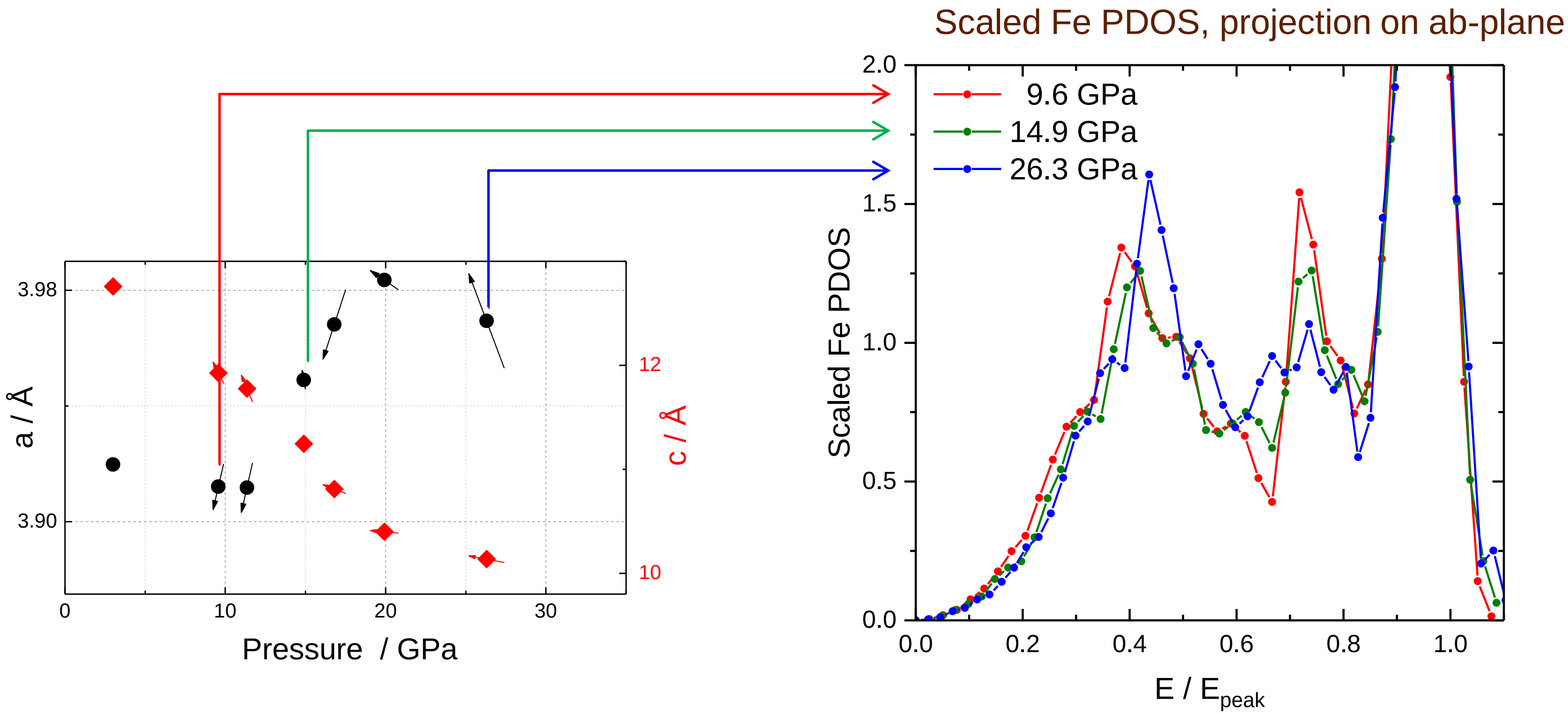


I.Sergueev, R. P. Hermann, K. Glazyrin, H.-C. Wille, I.Kantor, M. A. McGuire, A. S. Sefat, B. C. Sales, D. Mandrus, and R. Rüffer, unpublished

DESY

$BaFe_2As_2$. Combined X-ray and NIS study at HP

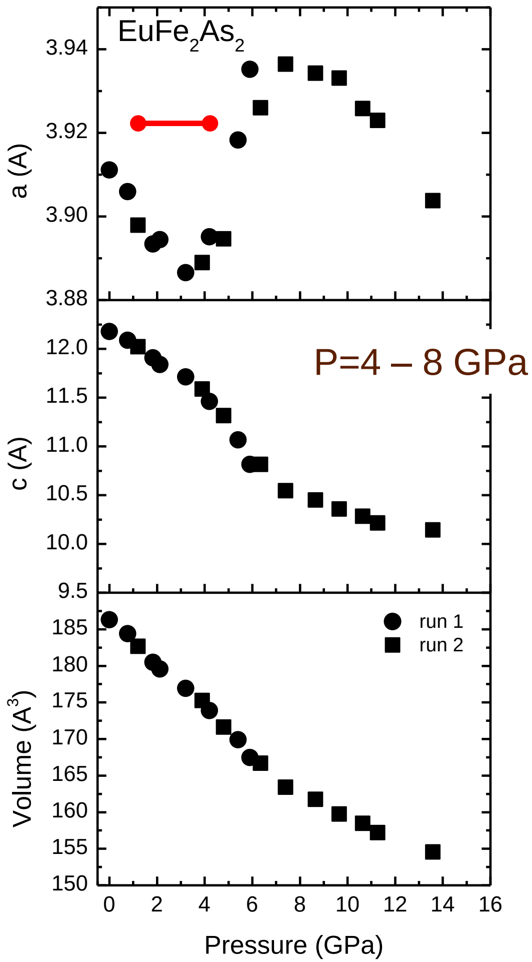
Sample: $BaFe_2As_2$ crystal in DAC with c-axis along diamond
Pressure medium: paraffin oil



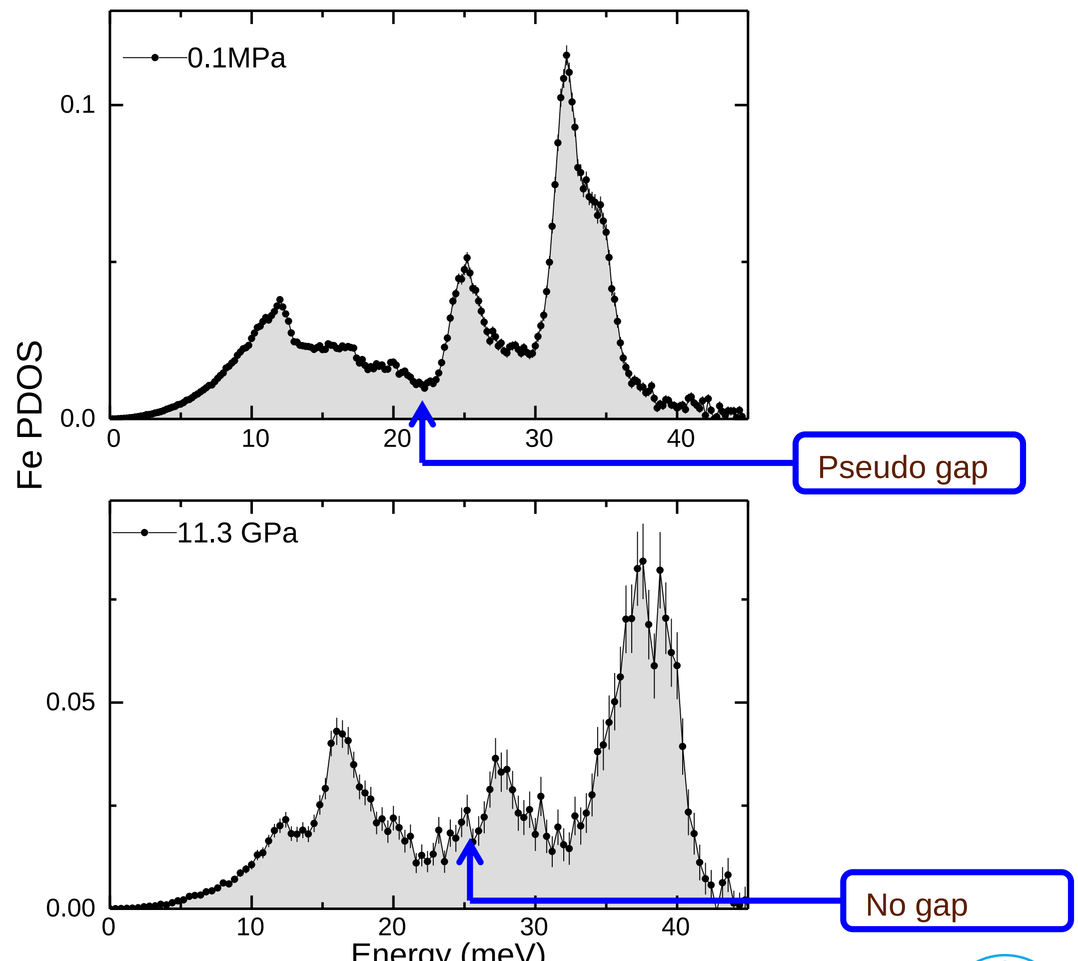
$EuFe_2As_2$. Pressure behaviour

X-ray diffraction,
P02, PETRAIII

Sample: $EuFe_2As_2$ poly crystal in DAC
Pressure medium: ethanol/methanol



^{57}Fe NIS at 296 K



I.Sergueev, R. P. Hermann, K. Glazyrin, U. Pelzer, M. Angst, W. Schweika, M. A. McGuire, A. S. Sefat, B. C. Sales, D. Mandrus, and R. Rüffer, unpublished

Conclusion

Assuming coupling between phonons and magnetic moment,
collapse of magnetism in 122 compounds occurs during T-cT transition

What about other families of Fe-superconductors (no T-cT transition is expected) ?

Demands for EBS:

- Beam size is NOT an issue
- Flux is always issue. However, it will not be significantly improved
- Better energy resolution is important in order to see small difference in phonon structure with small change of applied pressure. Monochromator with 0.1 meV energy resolution (spectrograph) would be important improvement.

Thank you for your attention