Nuclear Resonant Studies at High P,T

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Acknowledgments

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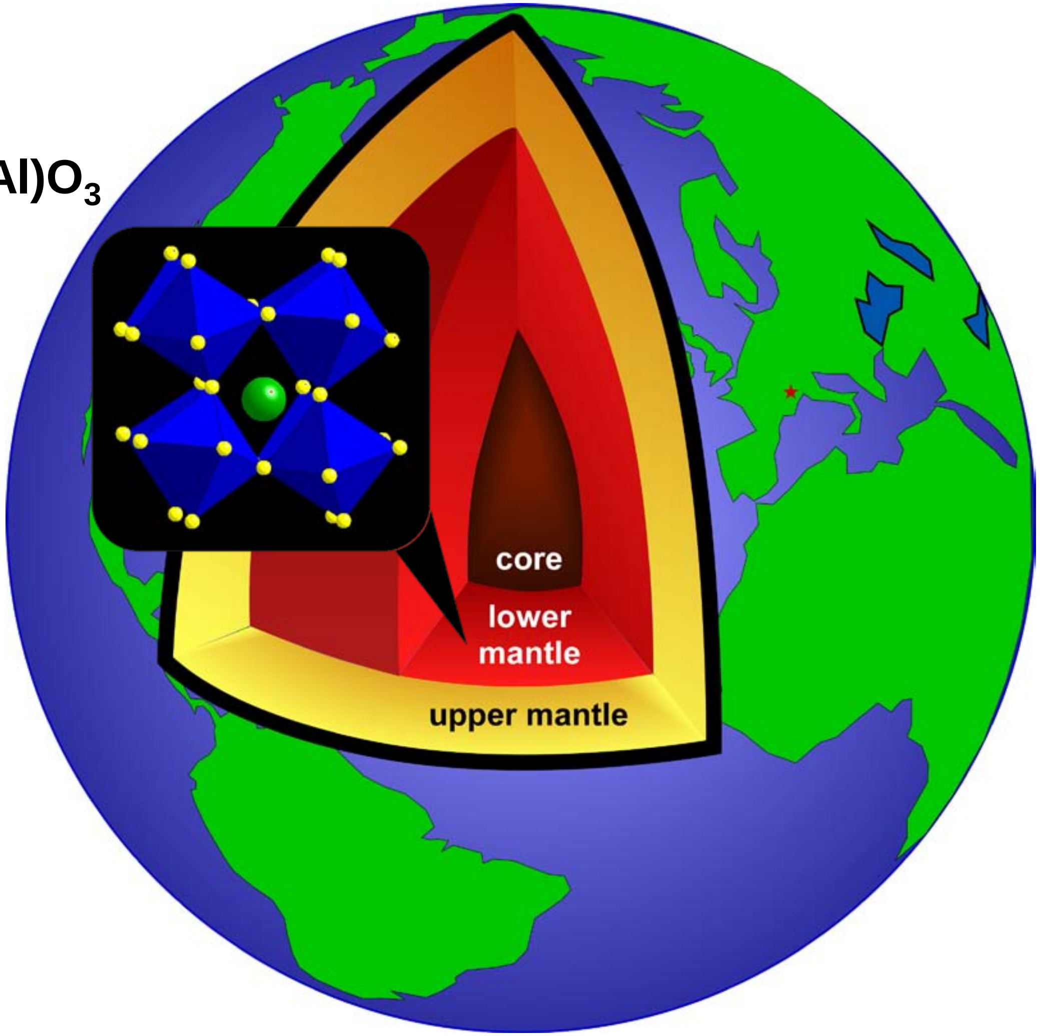
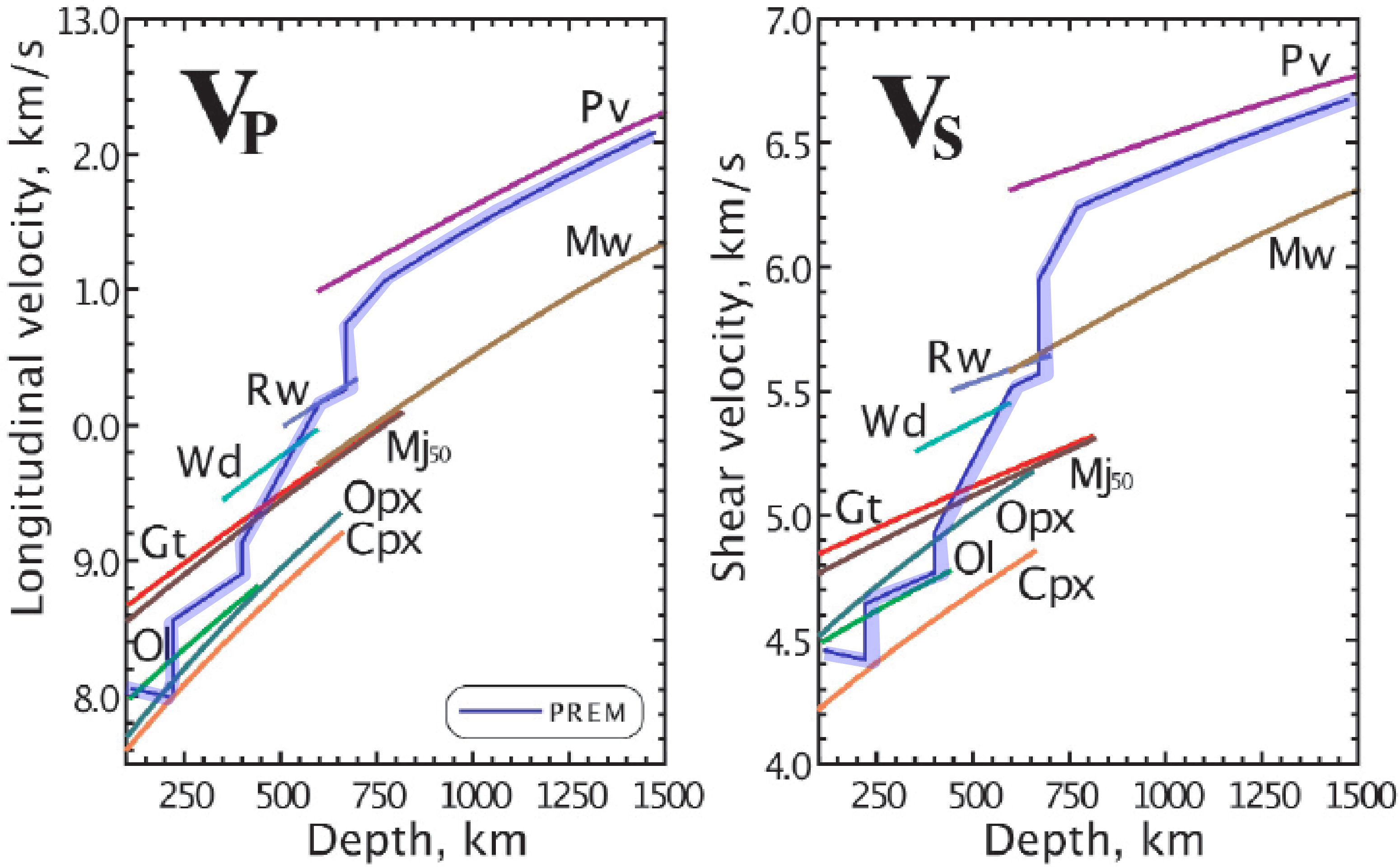
The Earth beneath our feet …

$(Mg,Fe)(Si,Al)O_3$
perovskite

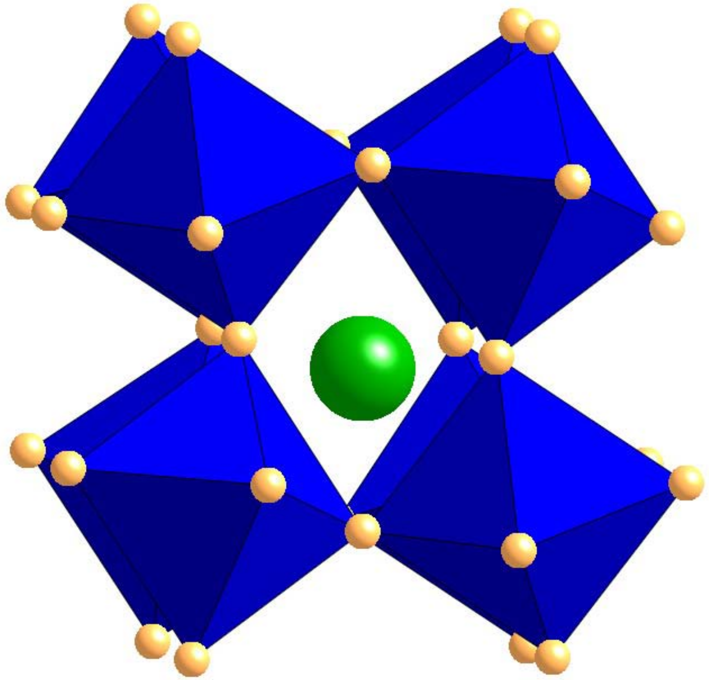


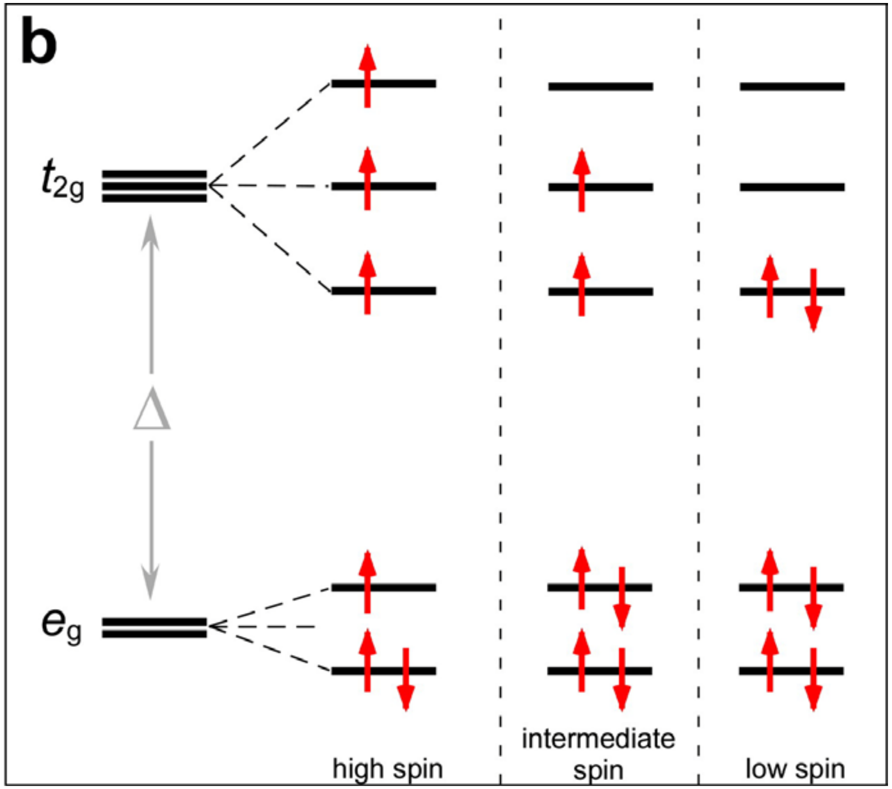
Modelling the Earth’s interior



Bass et al. (2008)

(Mg,Fe)(Si,Al)O_3 perovskite





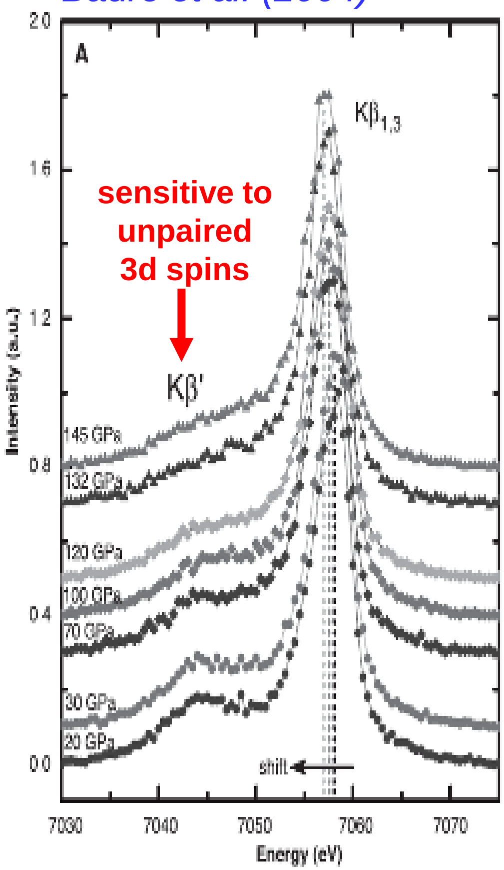
S=2 **S=1** **S=0**

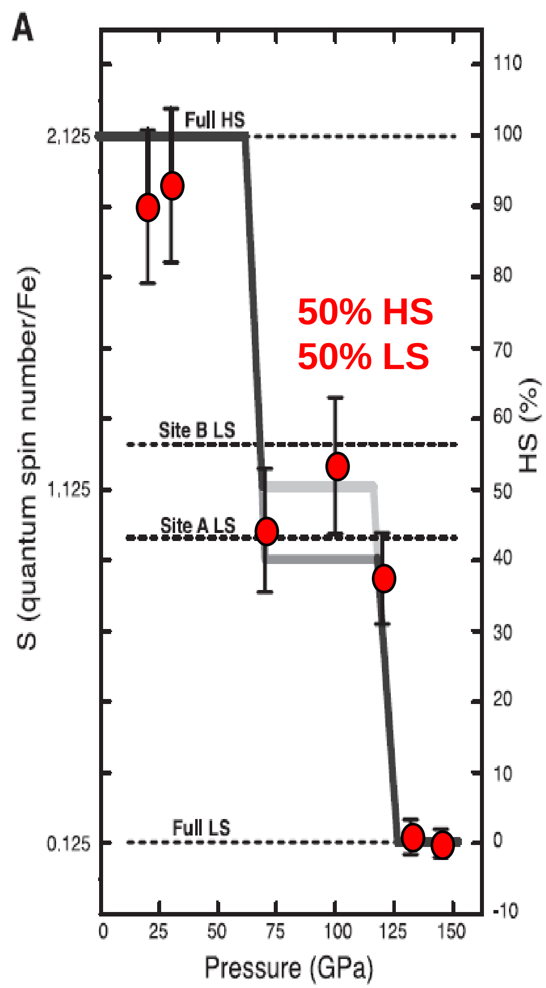
Previous XES data

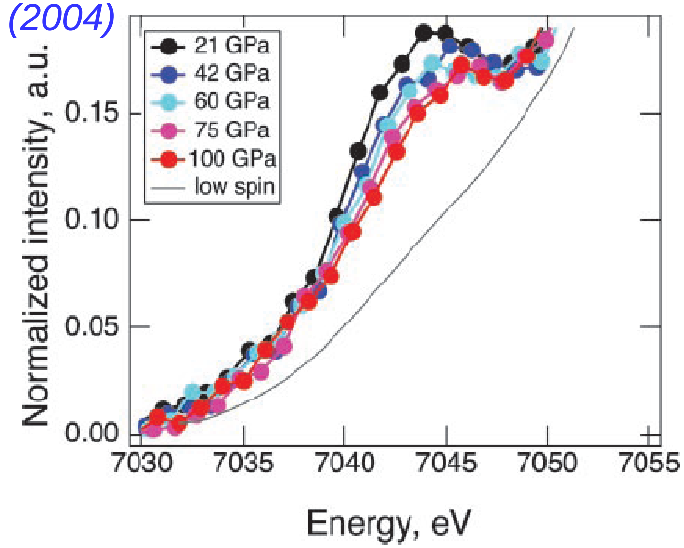
$Mg_{0.9}Fe_{0.1}SiO_3$ perovskite

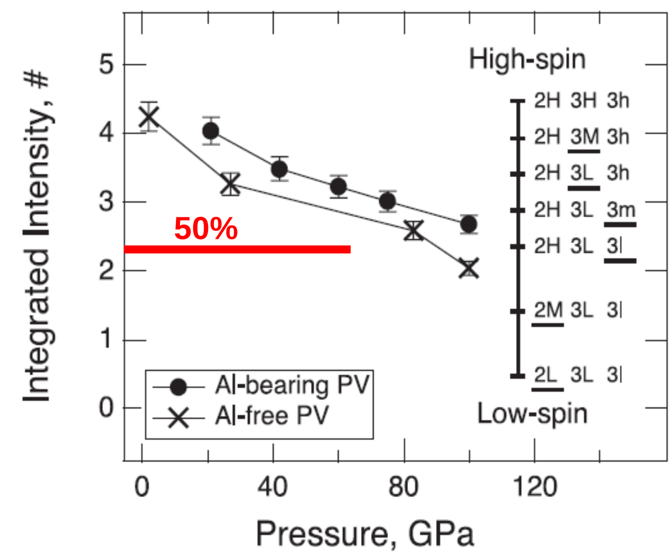
Li et al. (2004)

Badro et al. (2004)







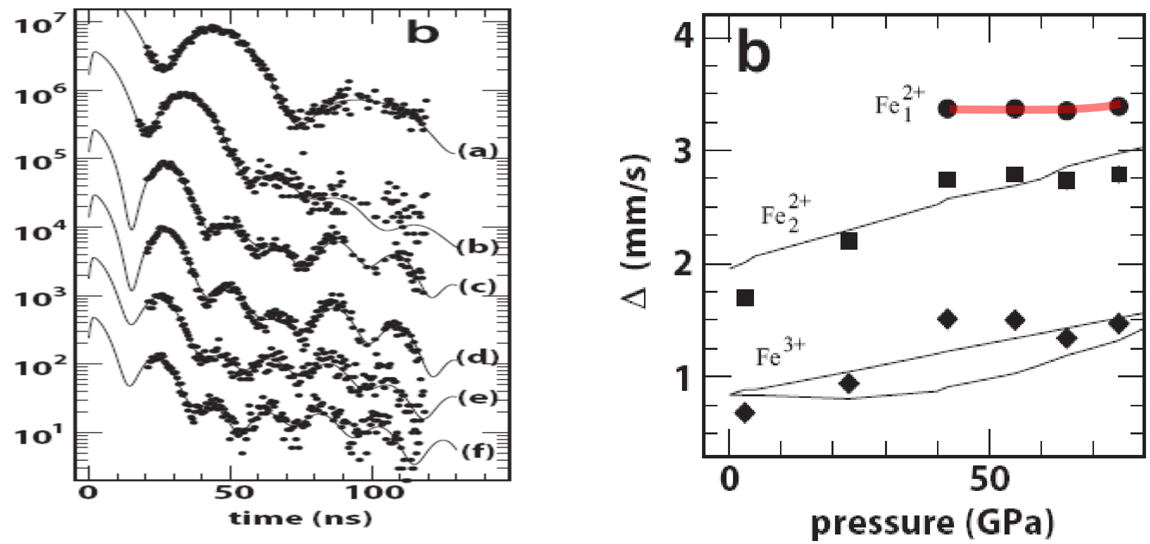


Previous NFS data

Jackson et al. (2005)

(Mg,Fe)SiO$_3$ pv

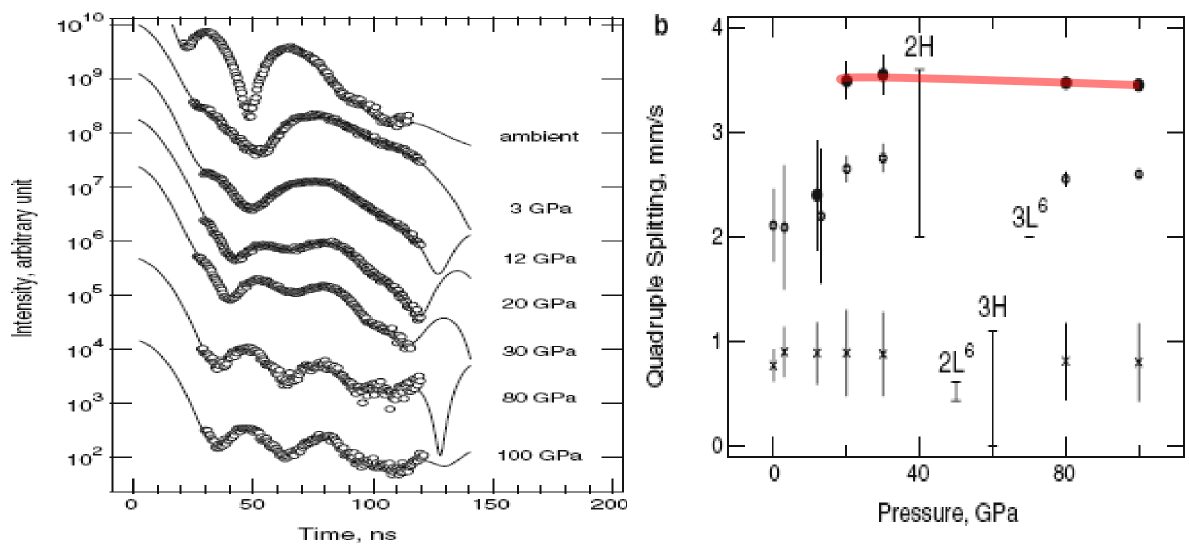
- not low-spin Fe^{2+}
- low-spin Fe^{3+}?



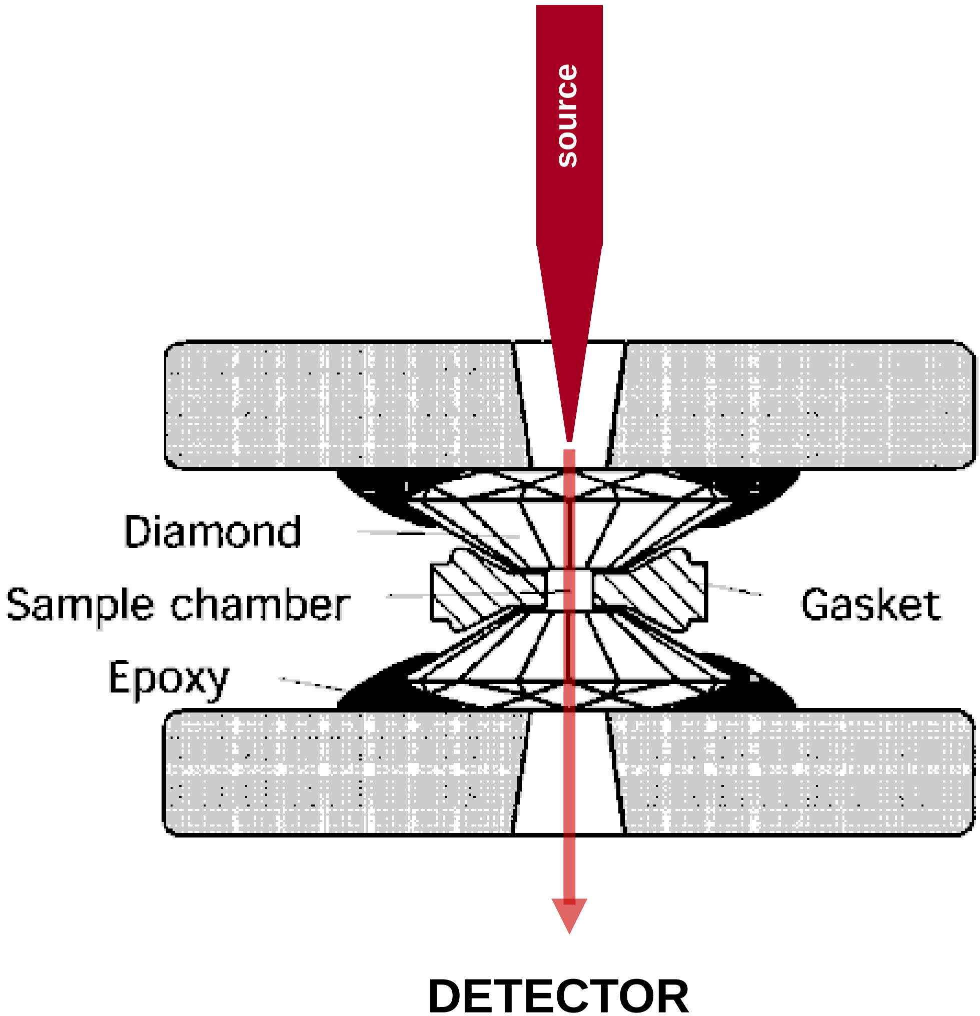
Li et al. (2006)

(Mg,Fe)(Si,Al)O$_3$ pv

- intermediate-spin Fe^{2+}?
- low-spin Fe^{3+}?

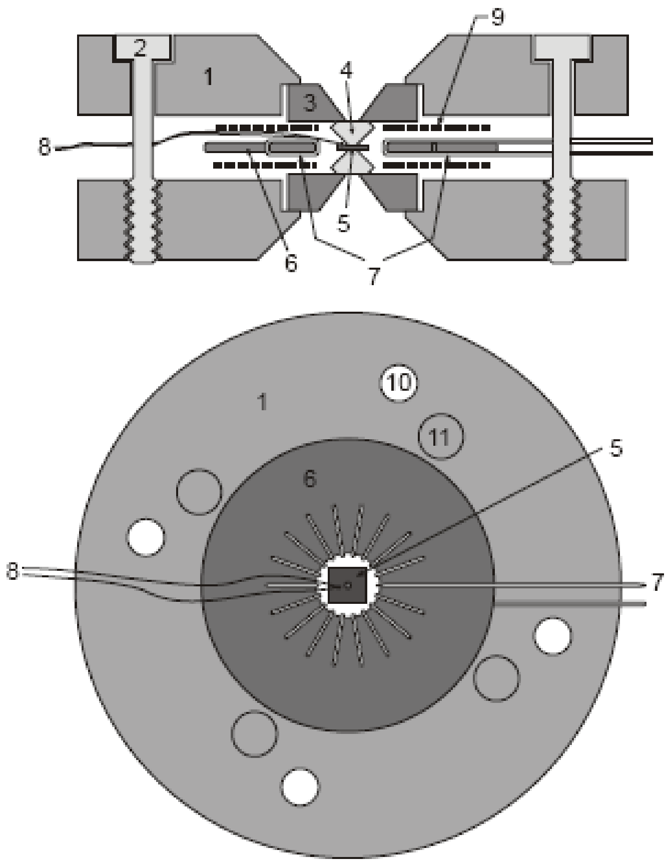


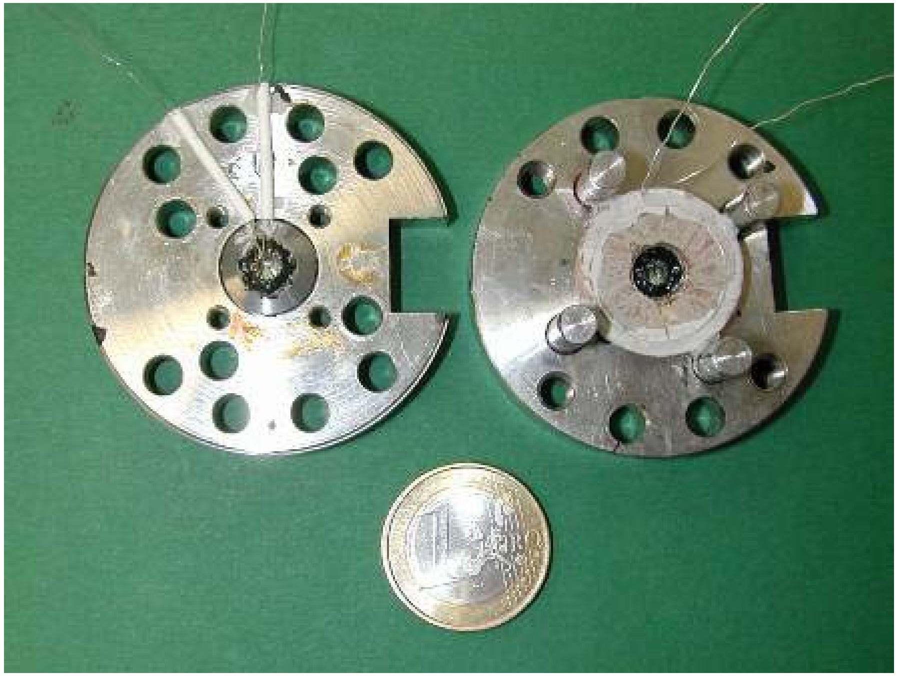
Mössbauer study at high P,T



- Re gasket with 100 µm hole
- 250 µm culet diamonds
- starting material $Fe_{0.12}Mg_{0.88}SiO_3$ and $Mg_{0.86}Fe_{0.14}Si_{0.98}Al_{0.02}O_3$
- 61% enriched in ^{57}Fe
- synthesis in multianvil press and/or by laser heating (LH) in DAC
- 16 different loadings of DAC
- 119 spectra 0-89 GPa, 300-800 K
- mostly LH between measurements
- collection time 1-2 days each

DAC external heater



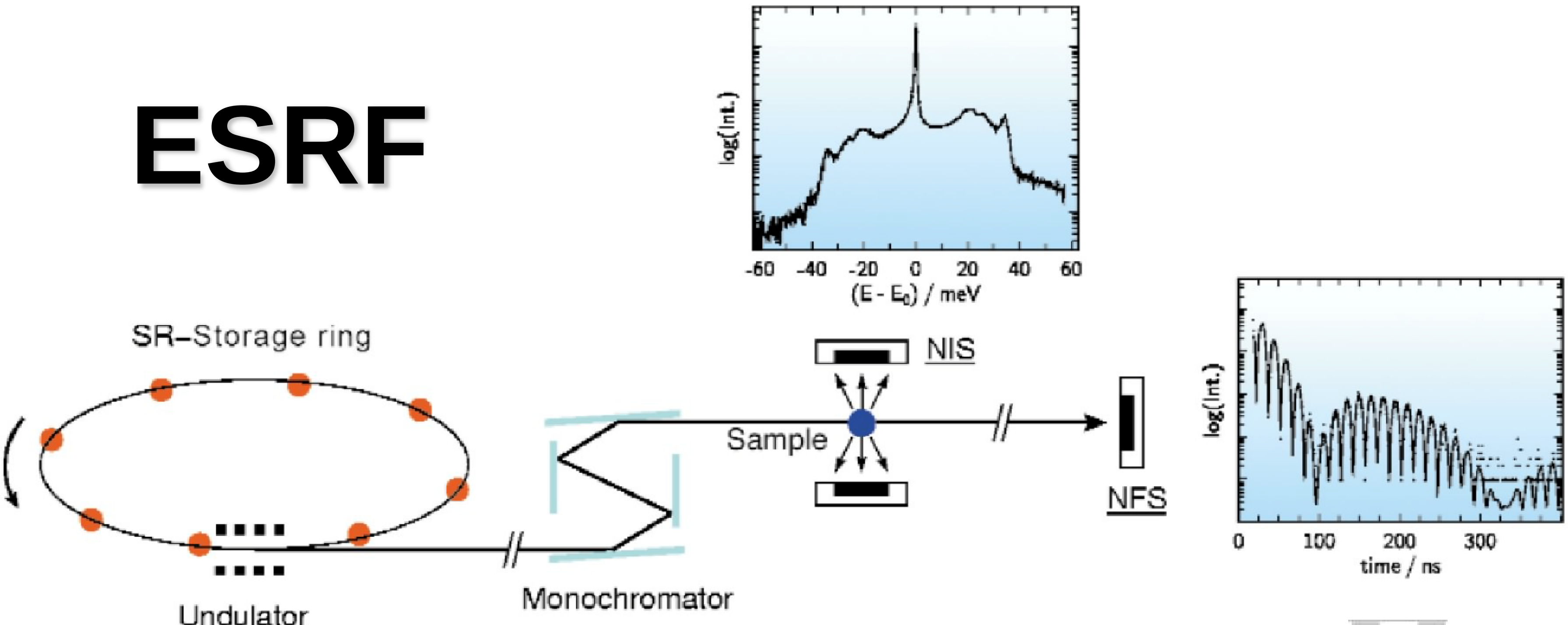


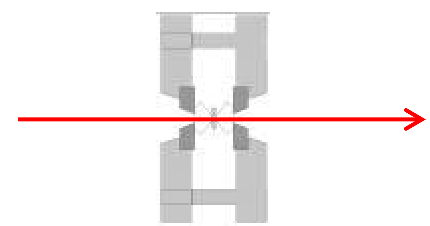
I. Kantor (2007) Ph.D. thesis

100 GPa = 1 x 10^6 bar

Nuclear forward scattering

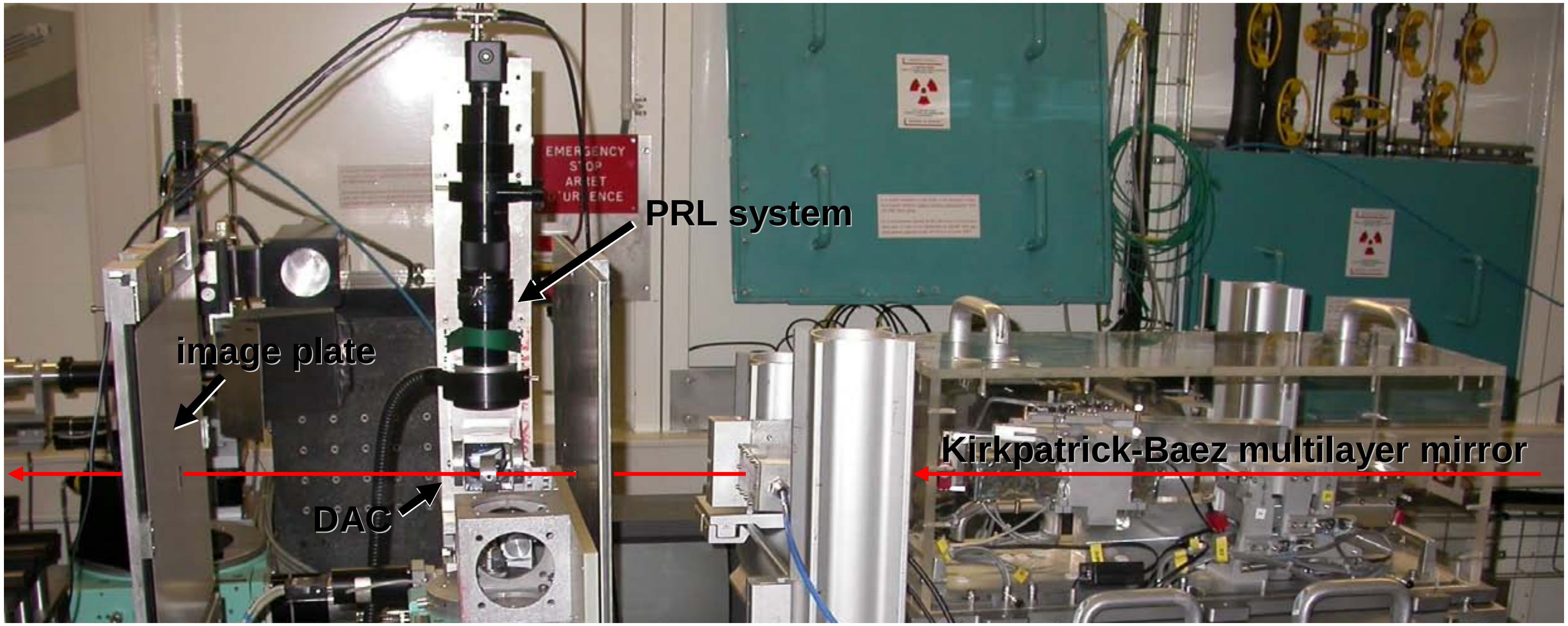
ESRF



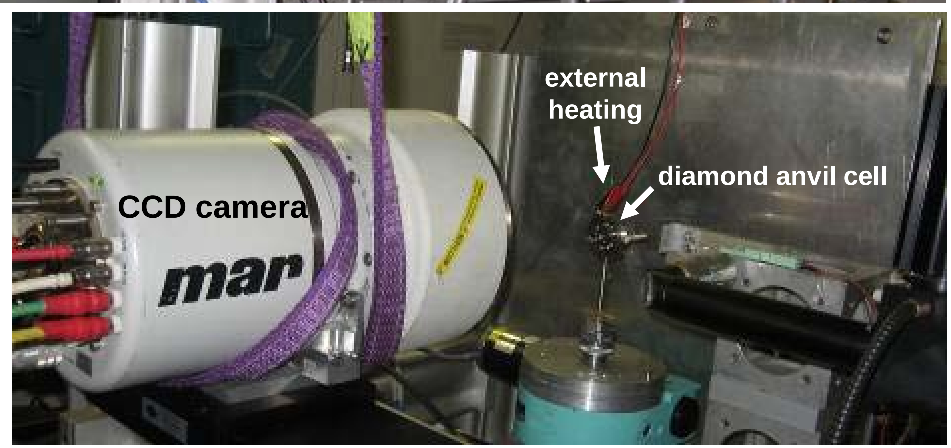


nuclear forward scattering

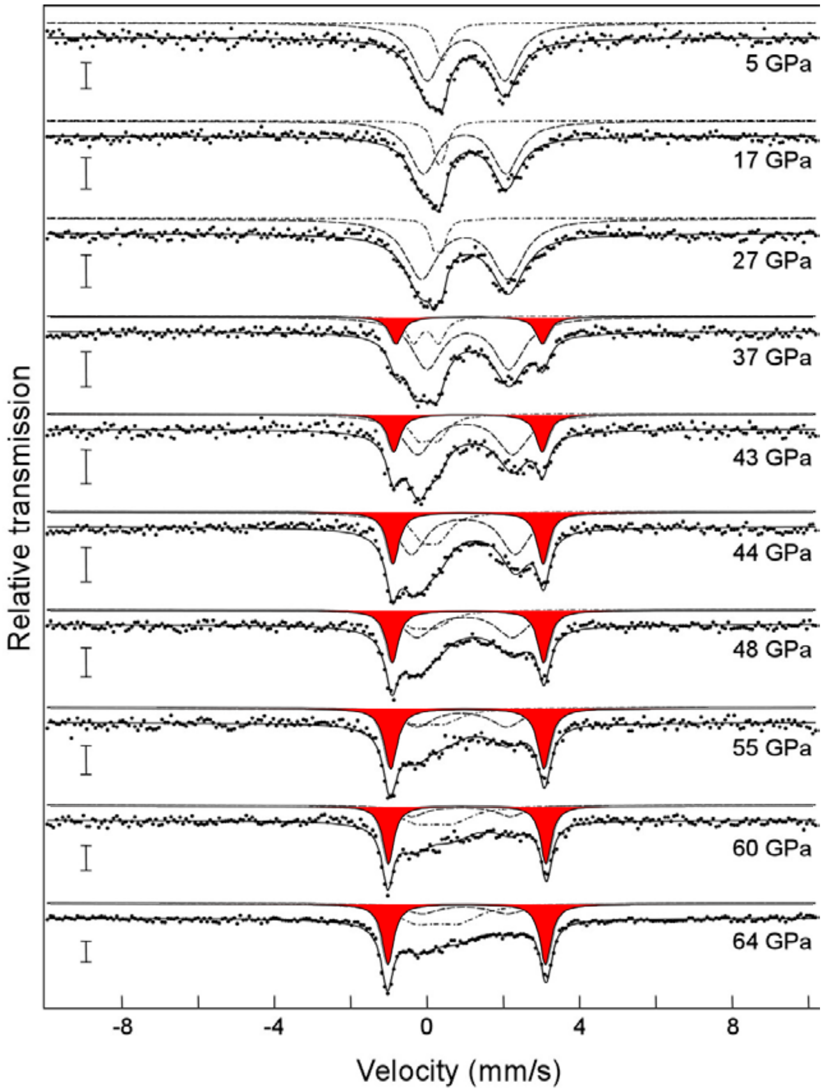
NFS study at high P,T



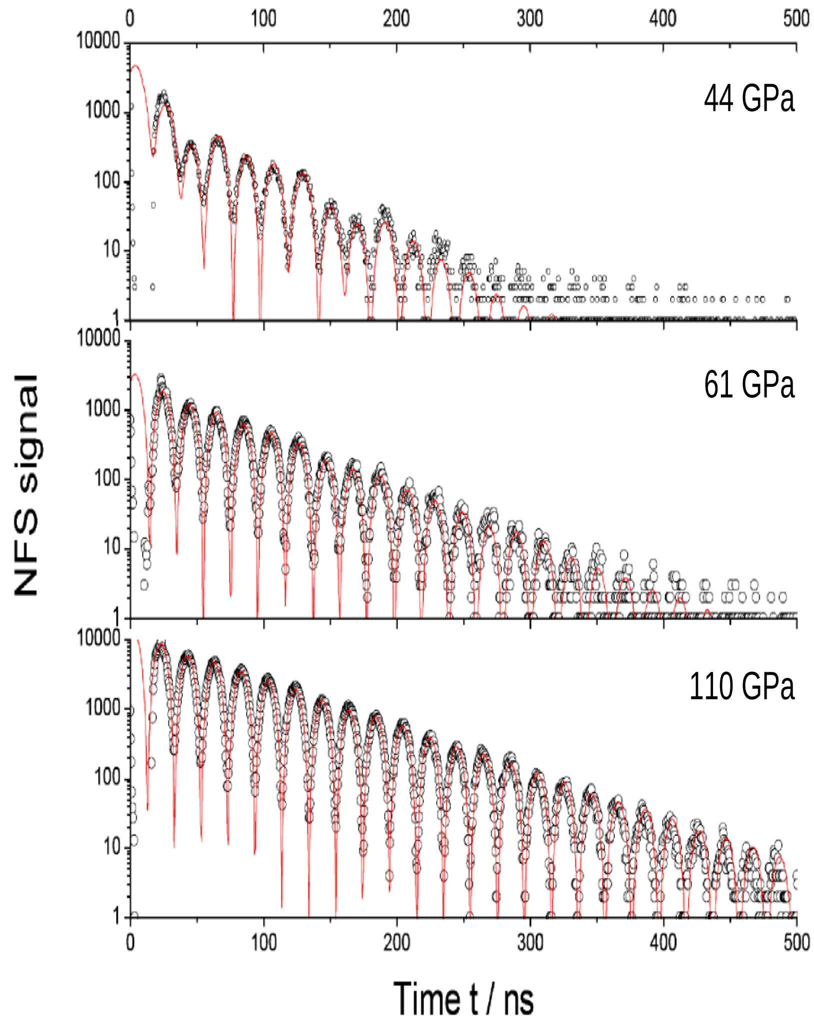
- ESRF ID18
- same DAC + sample as for MS
- 4 and 16 bunch mode
- 32 spectra to 110 GPa, 1000 K
- collection time 1-2 h each
- high-resolution XRD collected for same DAC at numerous P



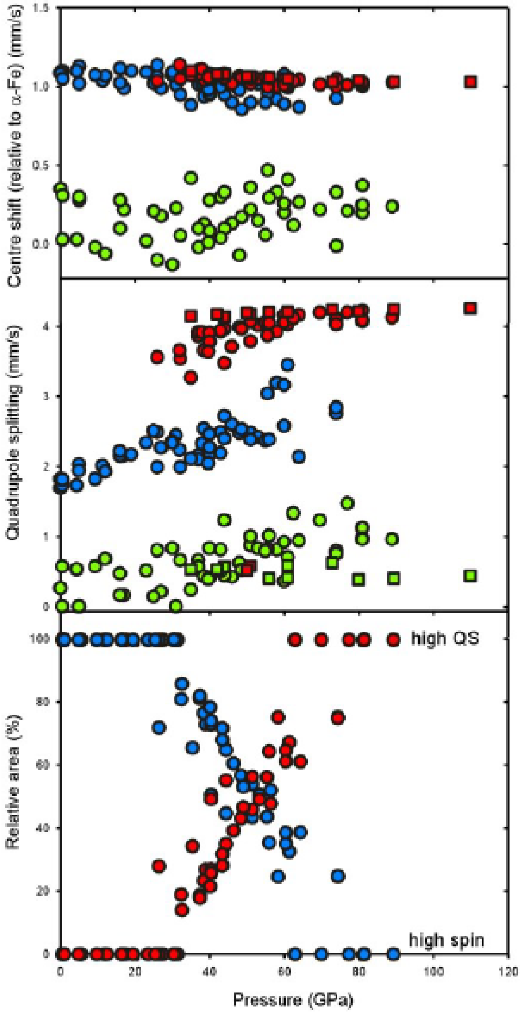
Room temperature spectra

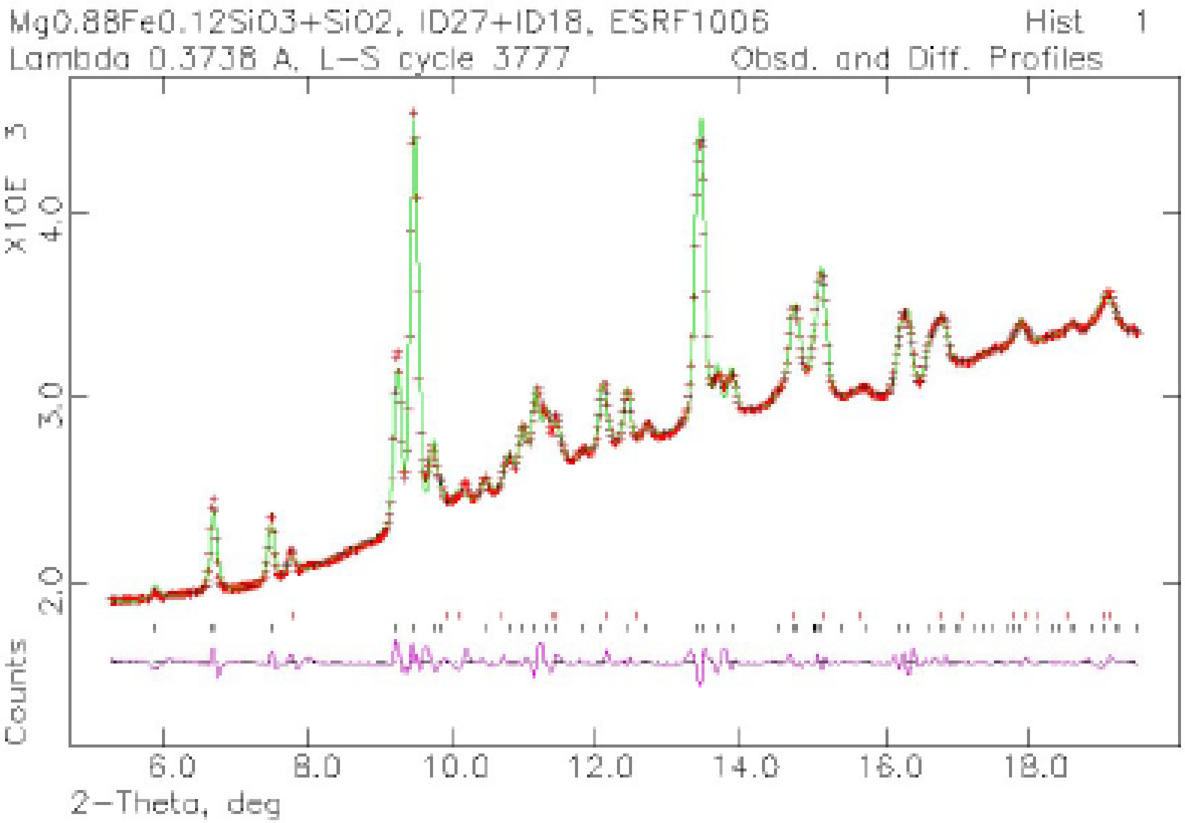


$Mg_{0.88}Fe_{0.12}SiO_3$ perovskite



Hyperfine parameters & crystal structure





Determination of spin state

$$S_T = \Sigma\, S_n \quad A_n$$

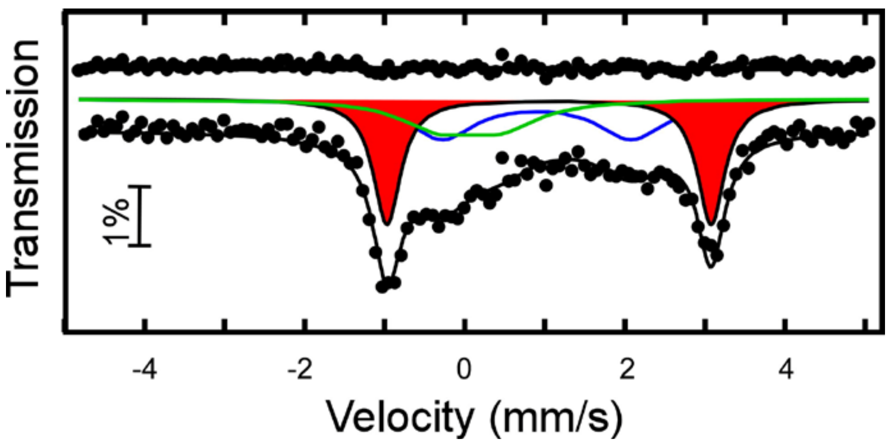
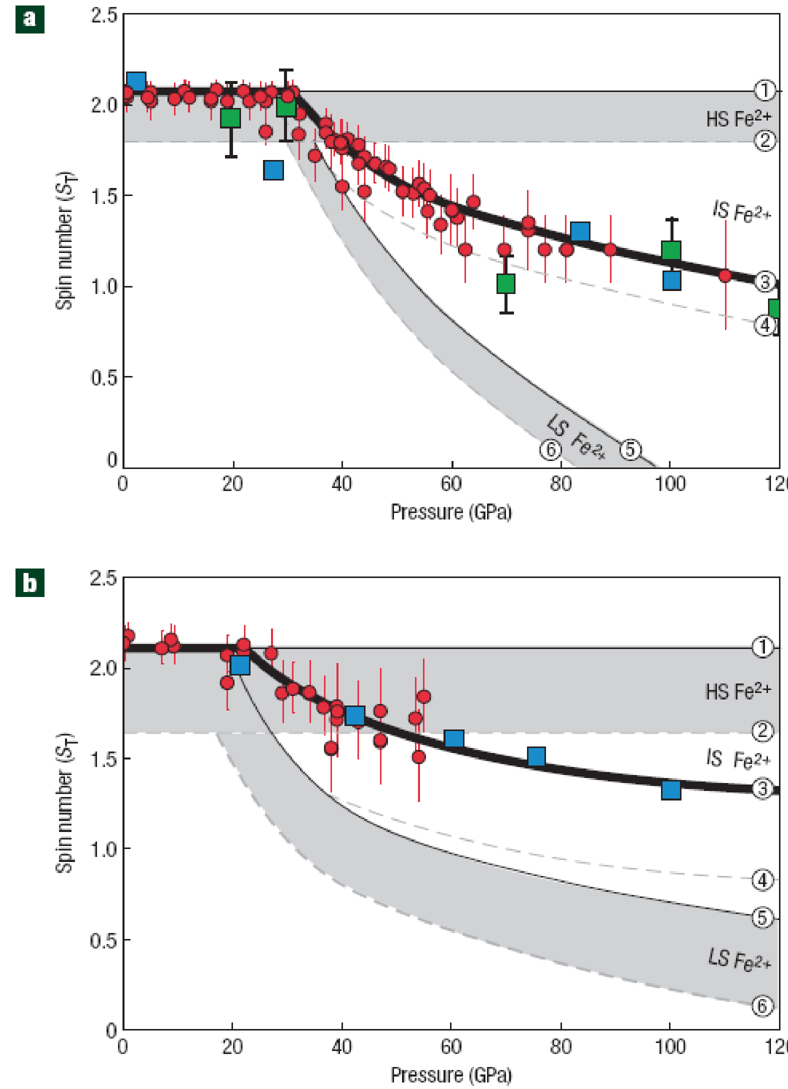
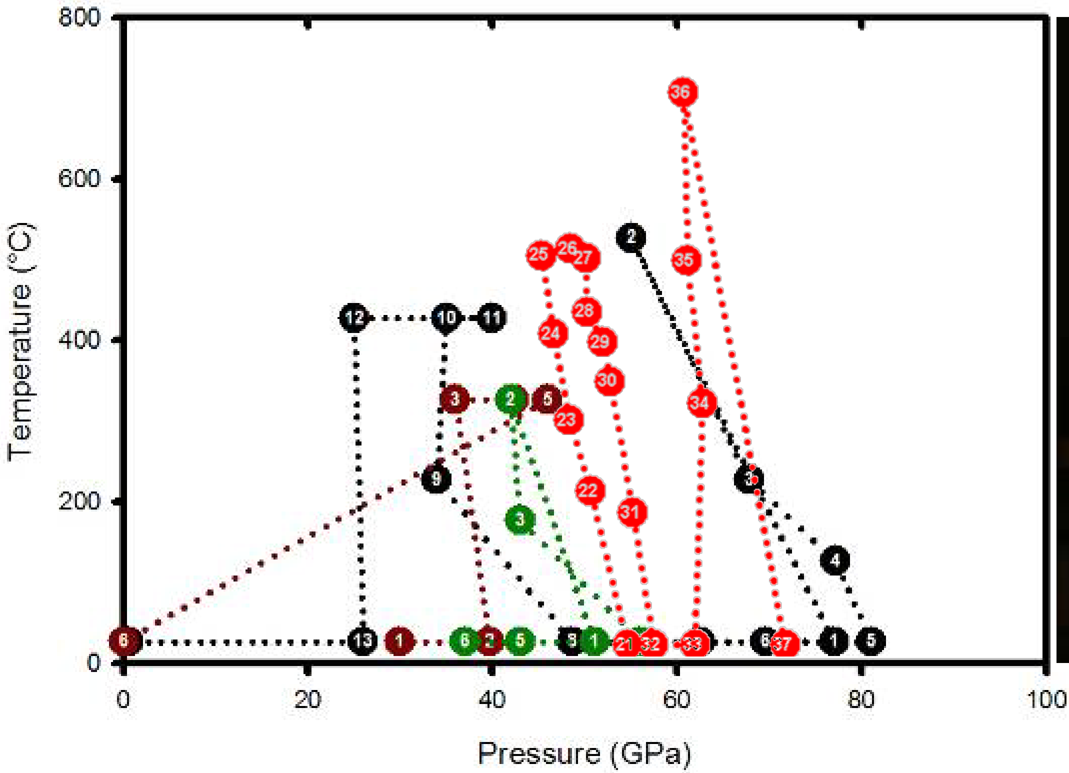


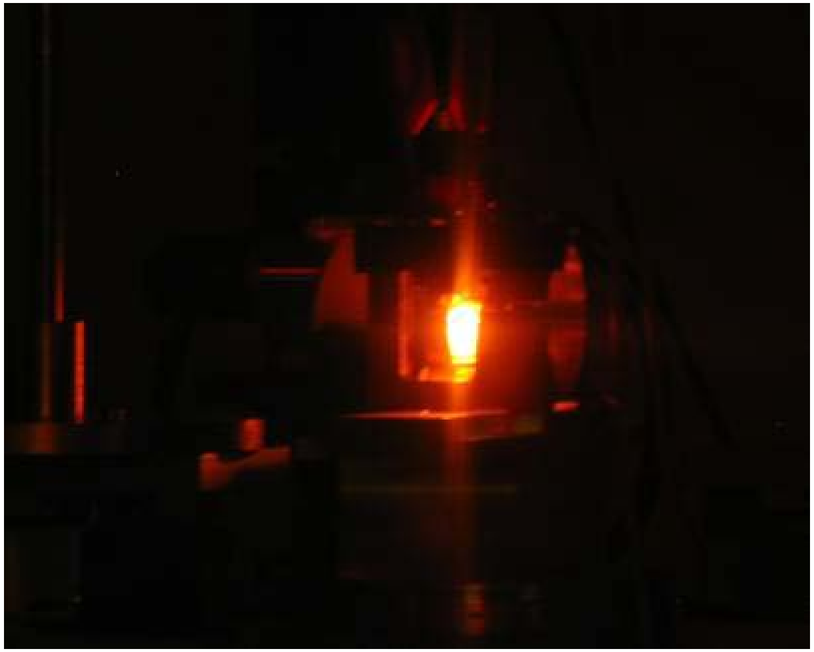
Table 1 Spin number assigned to each quadrupole doublet for total spin number calculation according to equation (1).

	Fe^{2+} QS < 3 mm s^{-1}	Fe^{2+} QS > 3.5 mm s^{-1} 'high QS'	Fe^{3+}
Model 1	2	2	5/2
Model 2	2	2	1/2
Model 3	2	1	5/2
Model 4	2	1	1/2
Model 5	2	0	5/2
Model 6	2	0	1/2

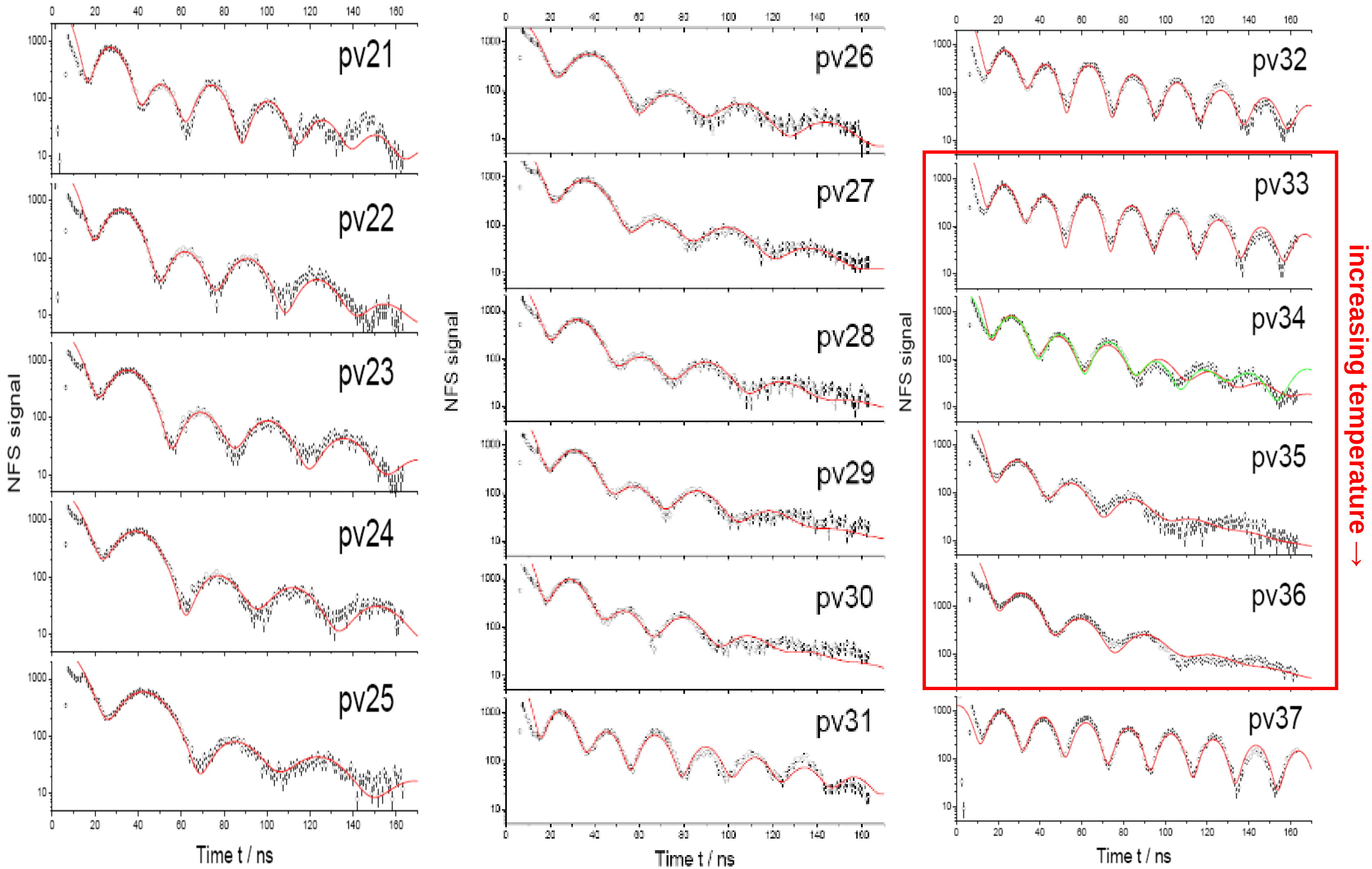


Pressure-temperature paths

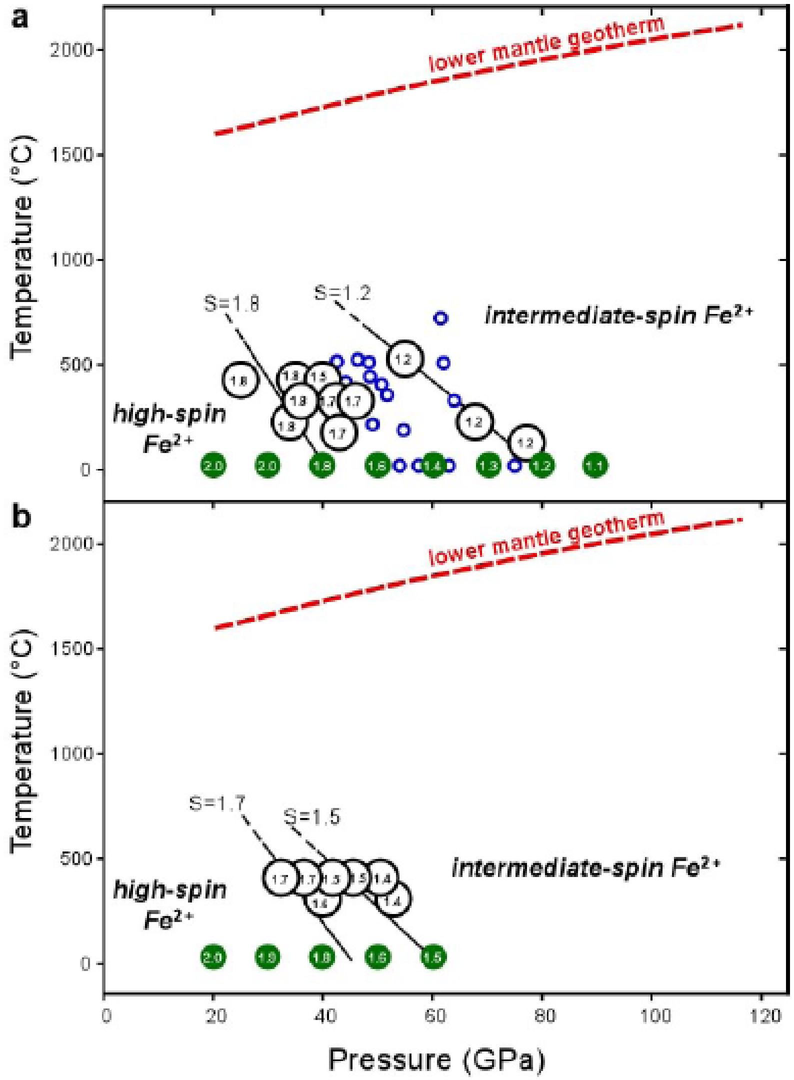




High temperature NFS spectra

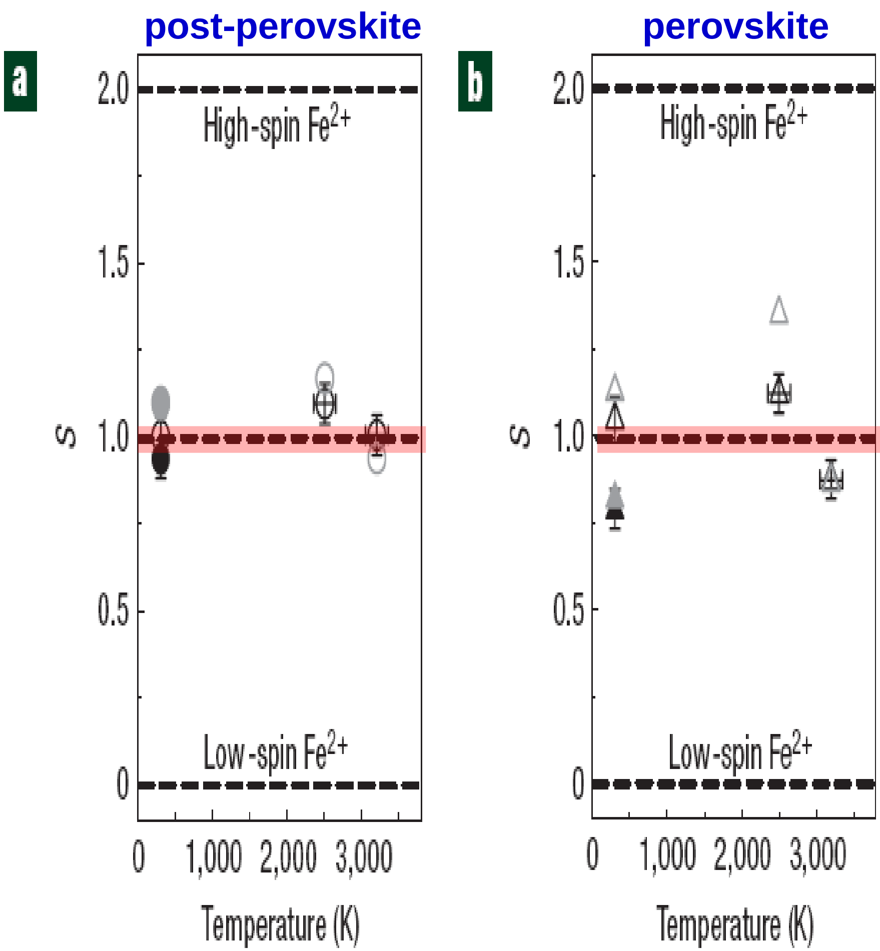


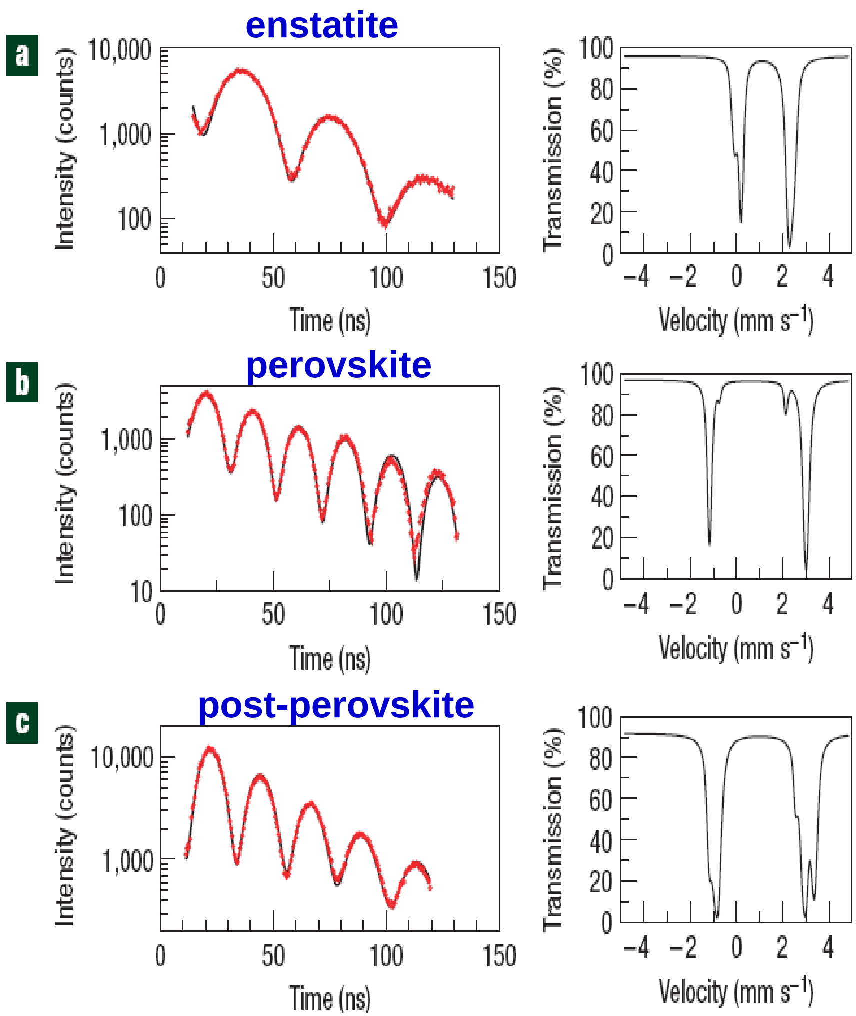
High P,T stability of intermediate-spin Fe^{2+}



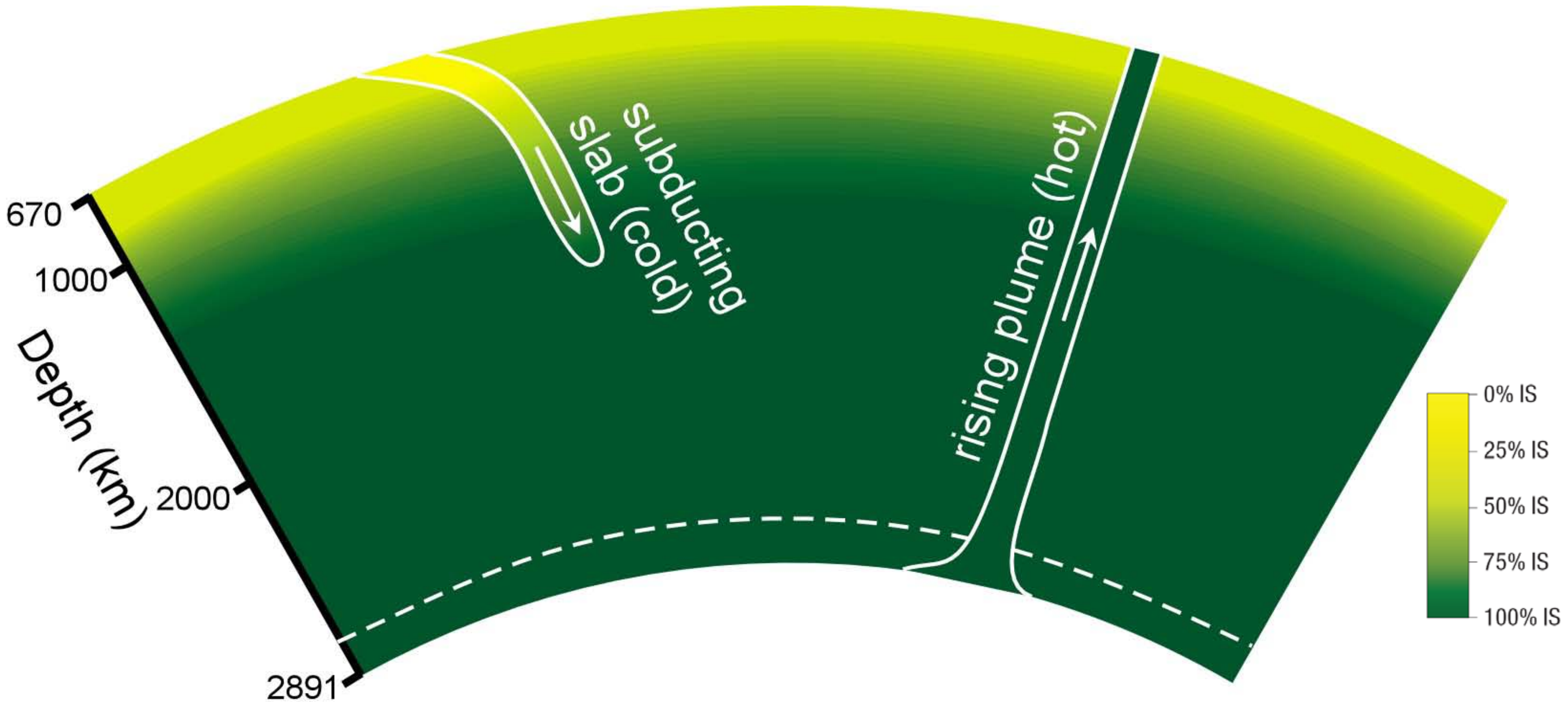
Intermediate spin Fe^{2+}: High-T XES & NFS

Lin et al. (2008)

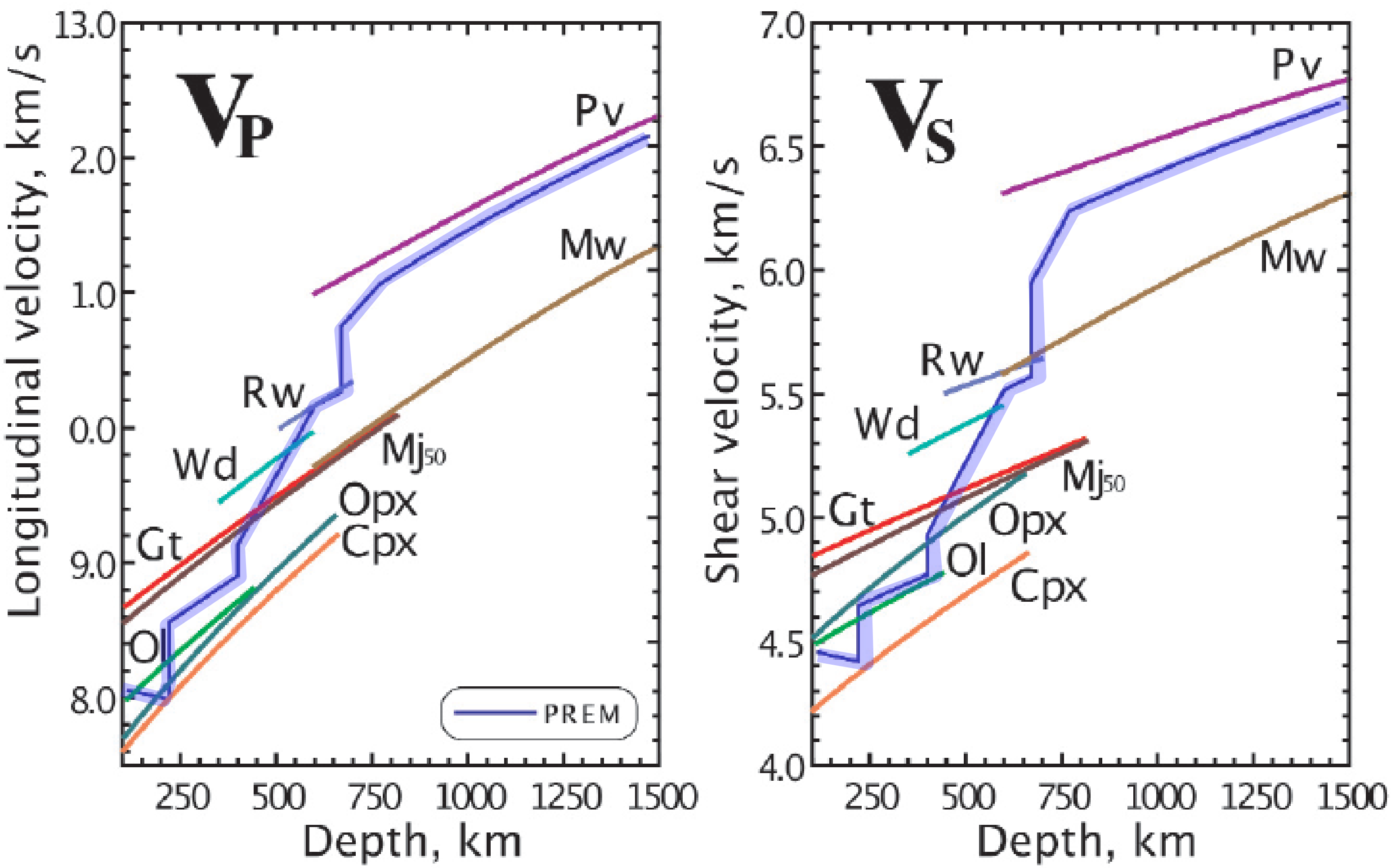




Spin transition zone in the lower mantle



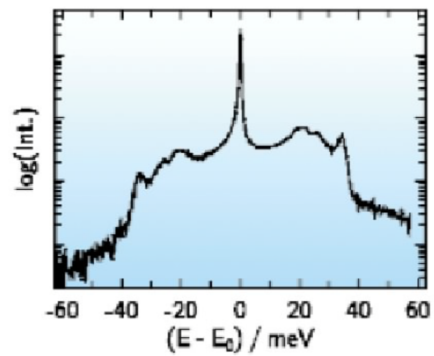
Modelling the Earth's interior

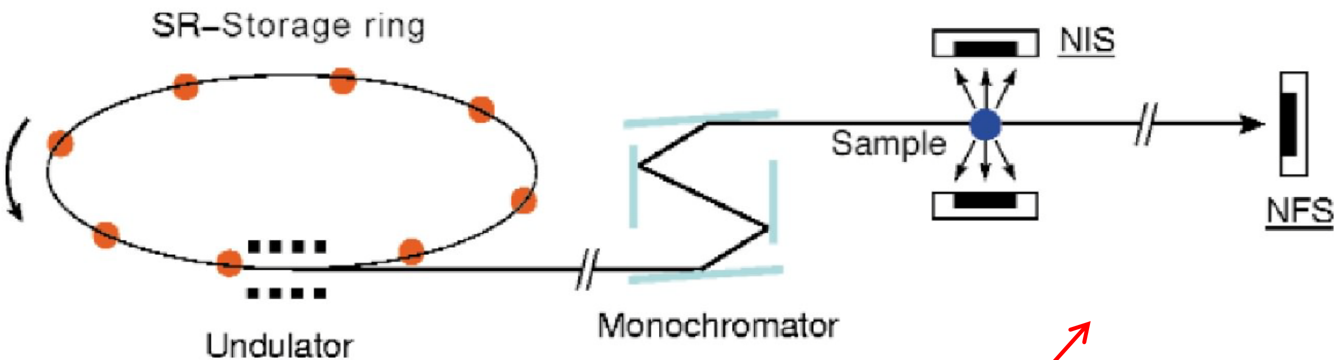


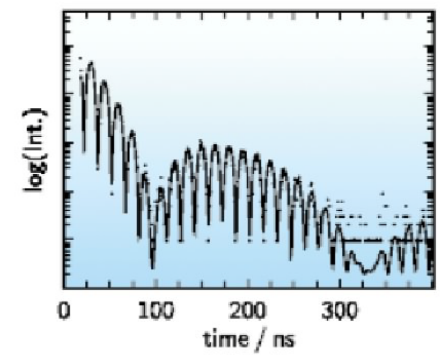
Bass et al. (2008)

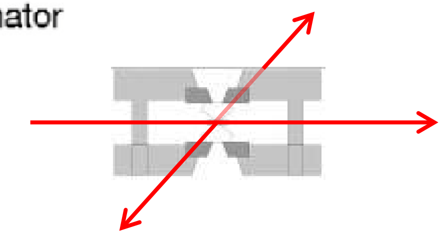
Nuclear inelastic scattering

ESRF



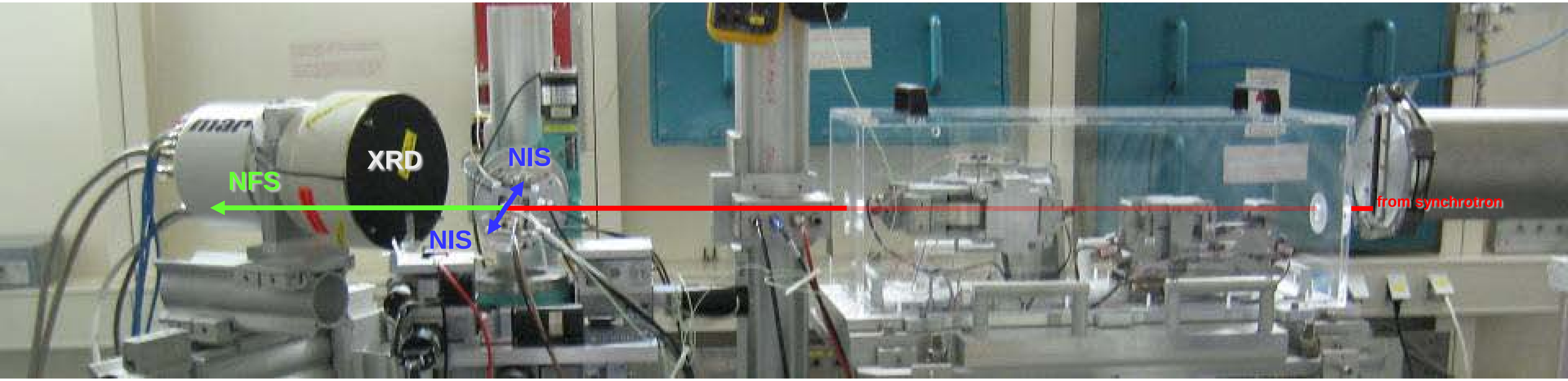


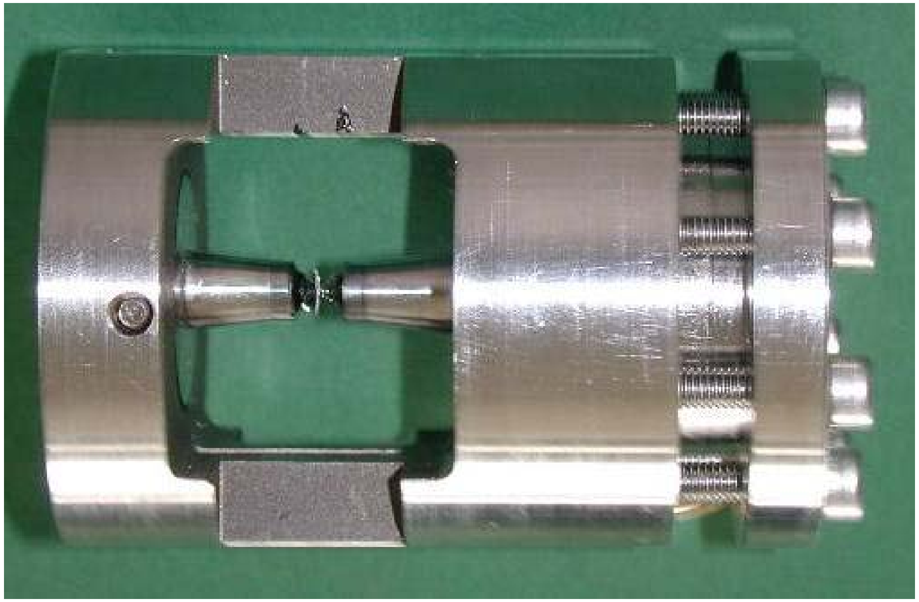


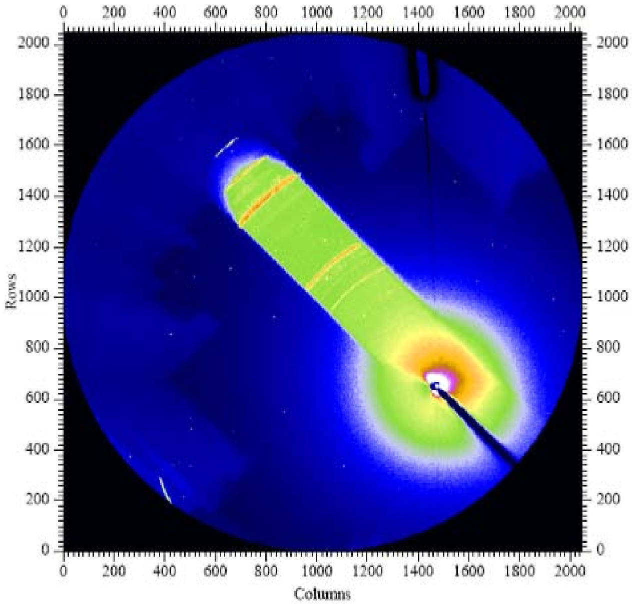


nuclear inelastic scattering

NFS/NIS/XRD general setup

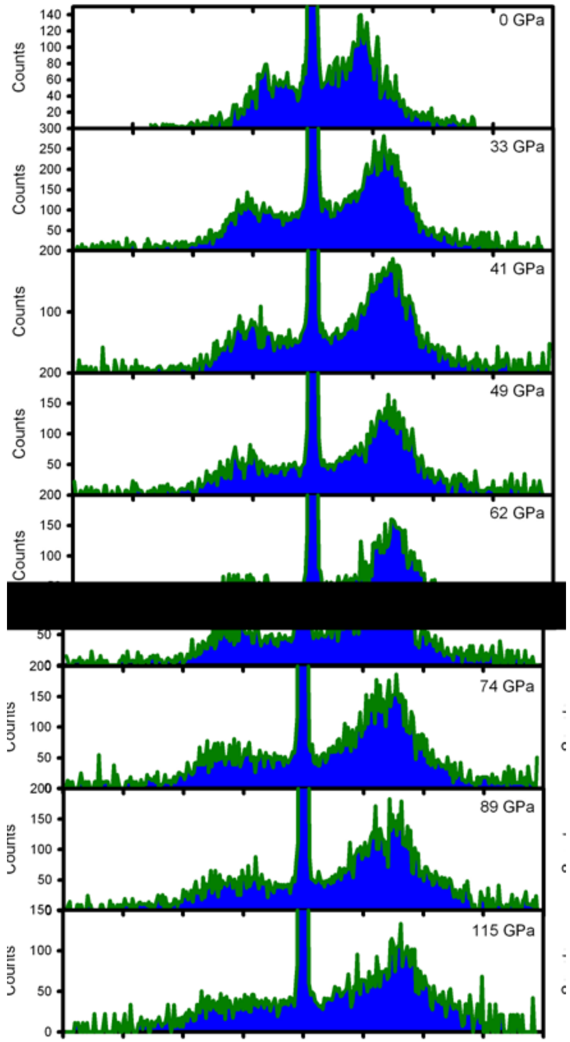




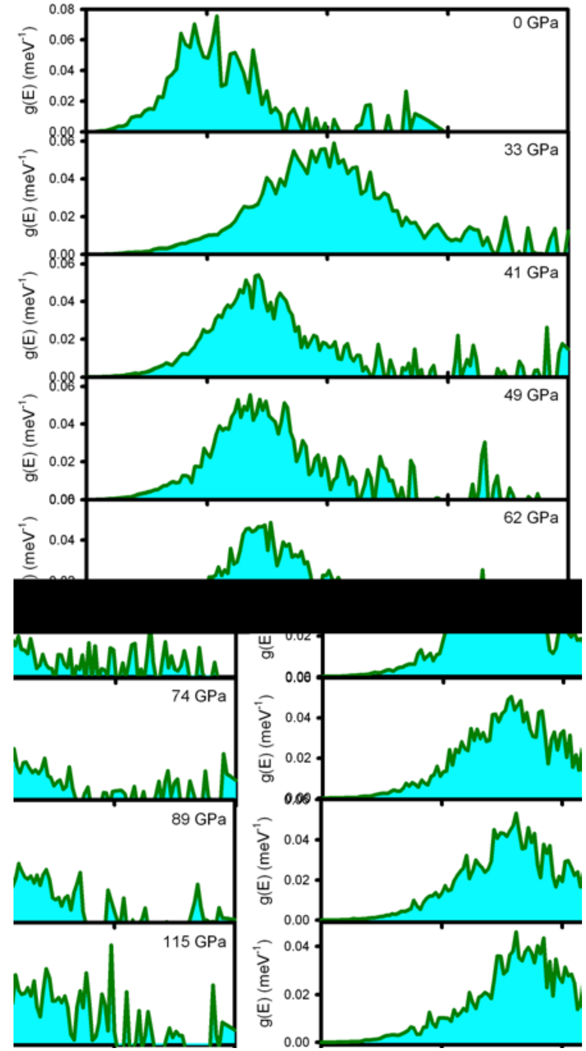


NIS data for $(Mg,Fe)SiO_3$ perovskite

nuclear inelastic absorption

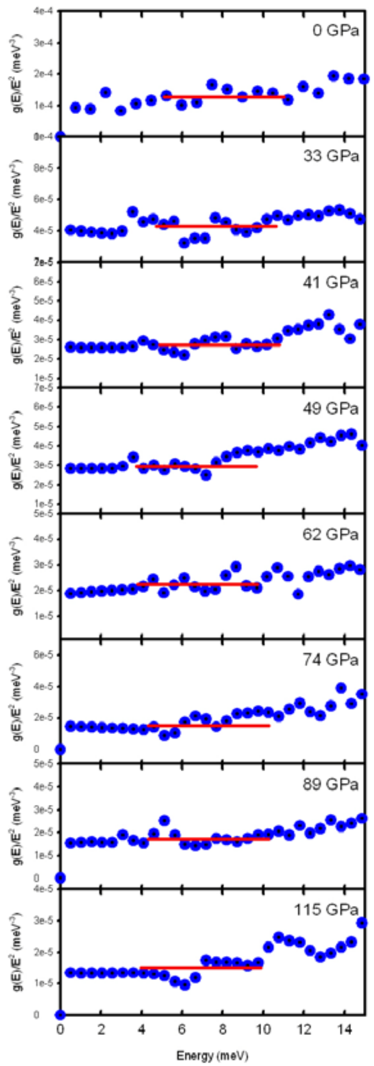


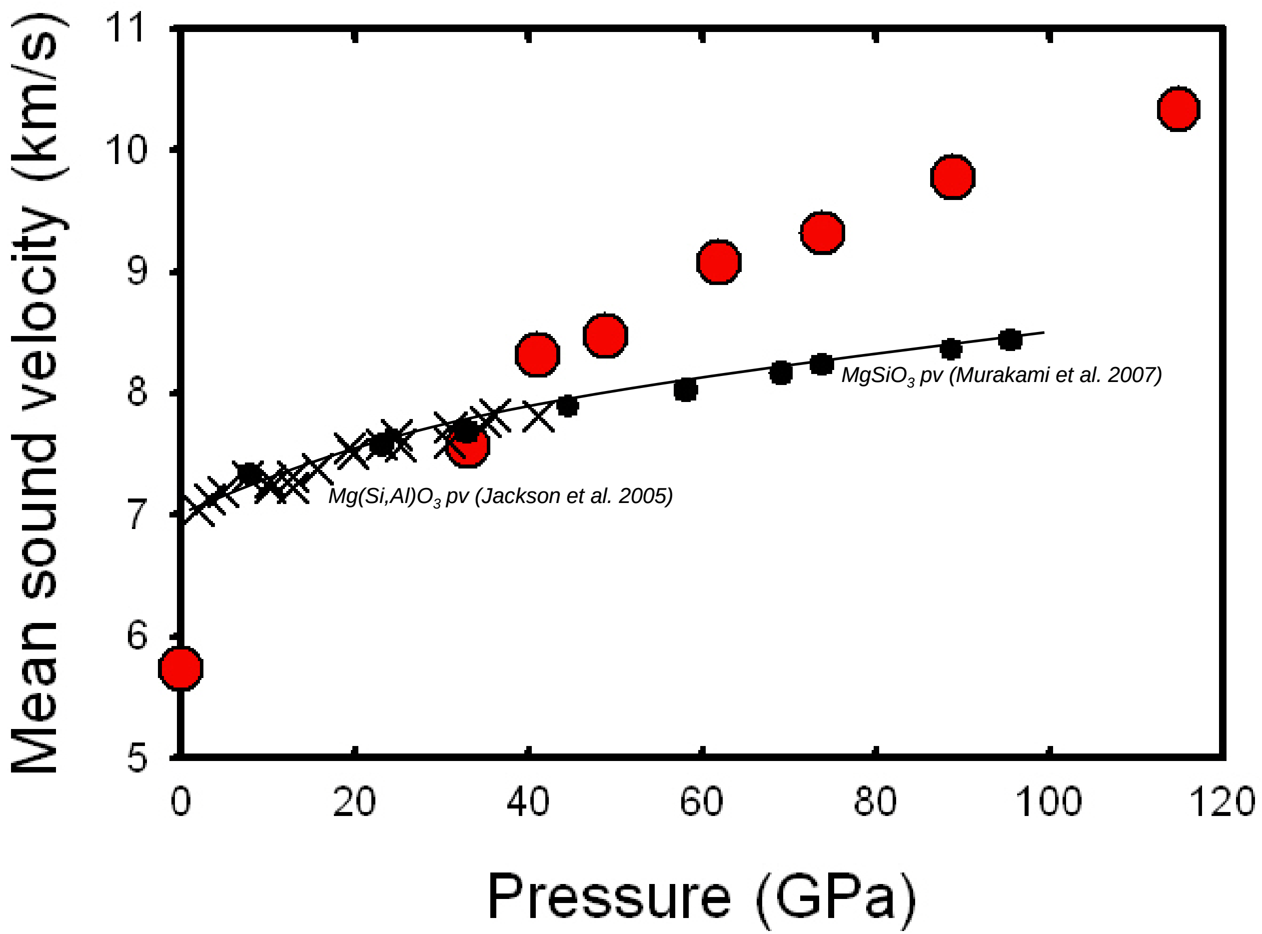
density of phonon states



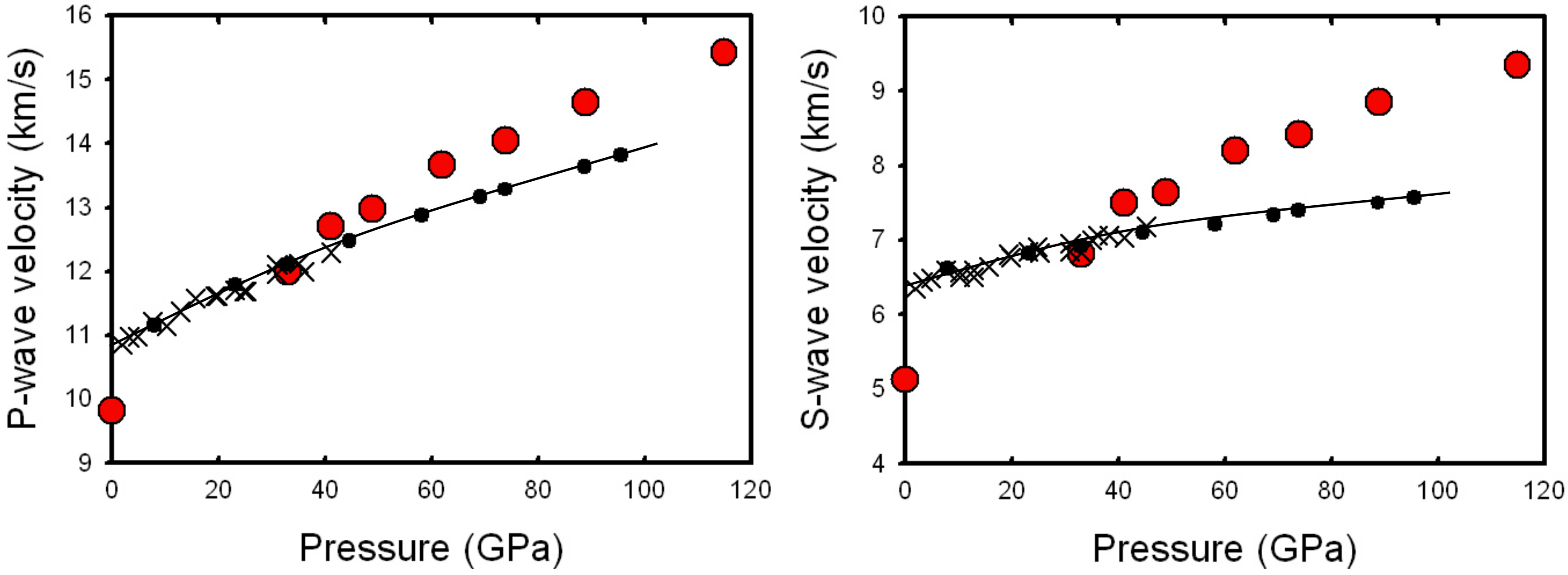
Mean sound velocity

reduced DOS





Seismic sound and shear wave velocities



Summary

- Mössbauer resonance methods can probe materials to at least 170 GPa and 1100 K

- NIS can directly probe properties available from direct geophysical measurements of Earth's interior

- Mössbauer (energy domain) and NFS (time domain) provide important complementary information