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Elasticity of (Mg,Fe)O Through the Spin Transition of Iron in the Lower Mantle

J. C. Crowhurst, *et al.*
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Changes in the electronic configuration of iron at high pressures toward a spin-paired state within host minerals ferropericlase and silicate perovskite may directly influence the seismic velocity structure of Earth's lower mantle. We measured the complete elastic tensor of ferropericlase, $(Mg_{1-x},Fe_x)O$ ($x = 0.06$), through the spin transition of iron, whereupon the elastic moduli exhibited up to 25% softening over an extended pressure range from 40 to 60 gigapascals. These results are fully consistent with a simple thermodynamic description of the transition. Examination of previous compression data shows that the magnitude of softening increases with iron content up to at least $x = 0.20$. Although the spin transition in (Mg,Fe)O is too broad to produce an abrupt seismic discontinuity in the lower mantle, the transition will produce a correlated negative anomaly for both compressional and shear velocities that extends throughout most, if not all, of the lower mantle.

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Spin Transition Zone in Earth's Lower Mantle

Jung-Fu Lin, *et al.*
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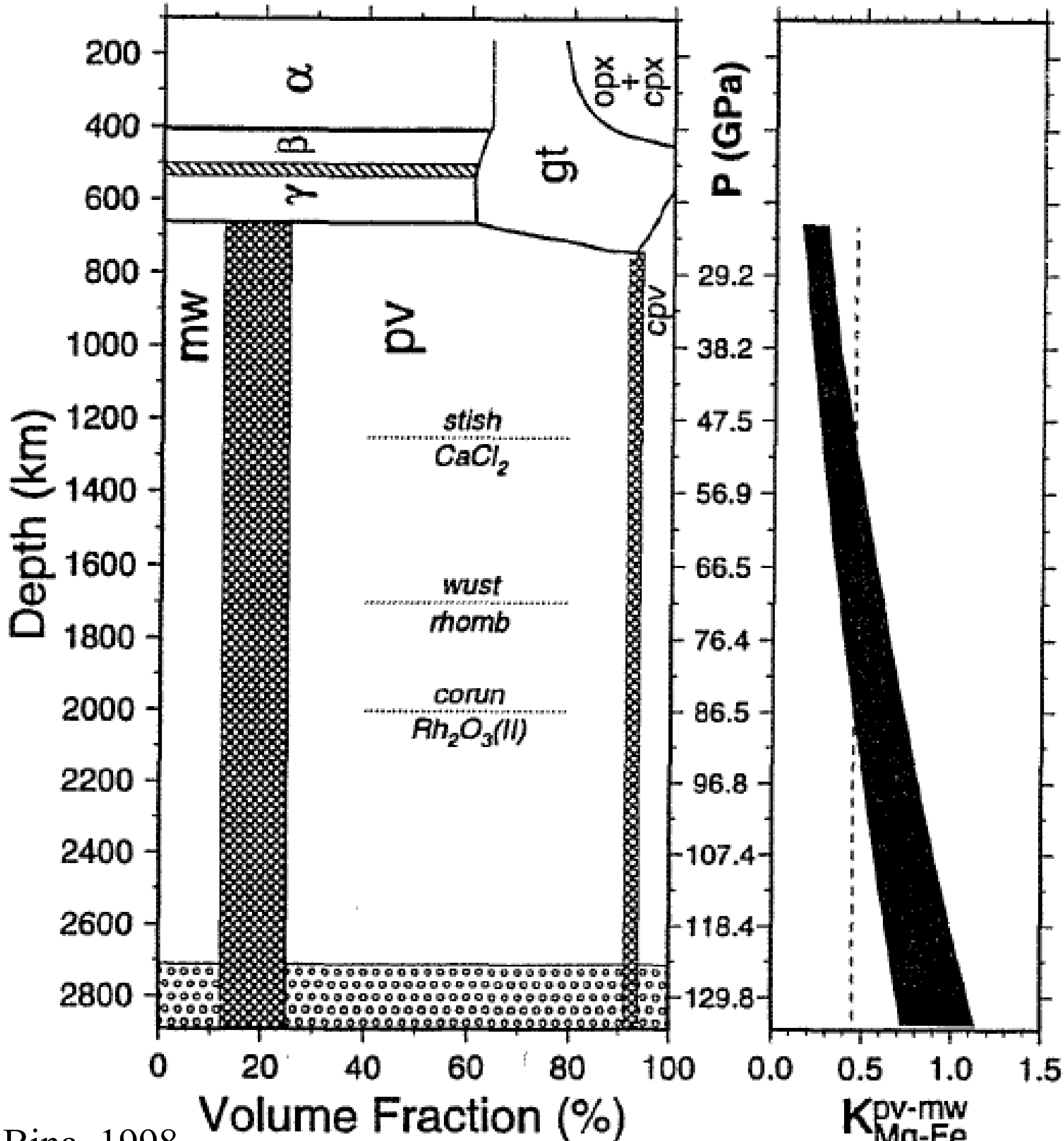
Mineral properties in Earth's lower mantle are affected by iron electronic states, but representative pressures and temperatures have not yet been probed. Spin states of iron in lower-mantle ferropericlase have been measured up to 95 gigapascals and 2000 kelvin with x-ray emission in a laser-heated diamond cell. A gradual spin transition of iron occurs over a pressure-temperature range extending from about 1000 kilometers in depth and 1900 kelvin to 2200 kilometers and 2300 kelvin in the lower mantle. Because low-spin ferropericlase exhibits higher density and faster sound velocities relative to the high-spin ferropericlase, the observed increase in low-spin (Mg,Fe)O at mid-lower mantle conditions would manifest seismically as a lower-mantle spin transition zone characterized by a steeper-than-normal density gradient.

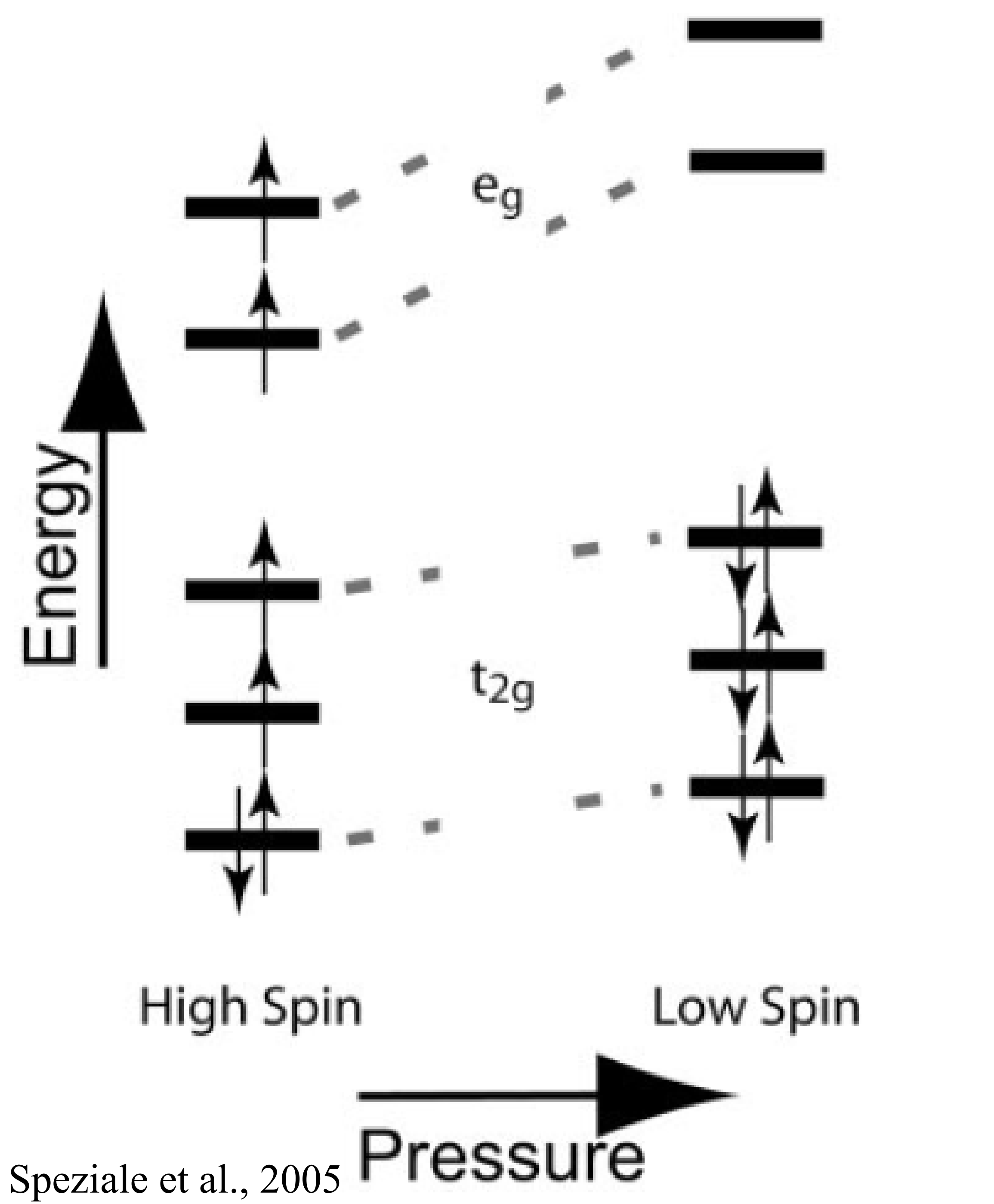
In 1960 **W. S. Fyfe** proposed that the effect of high pressure deep inside the Earth’s mantle may be to collapse the atomic orbitals of iron from the high-spin to the low-spin state.

This transition would represent a major change in chemical-bonding character for iron, with predictions suggesting as much as a 45% collapse in the ionic volume of ferrous iron in silicates and oxides (Shannon & Prewitt, 1969).

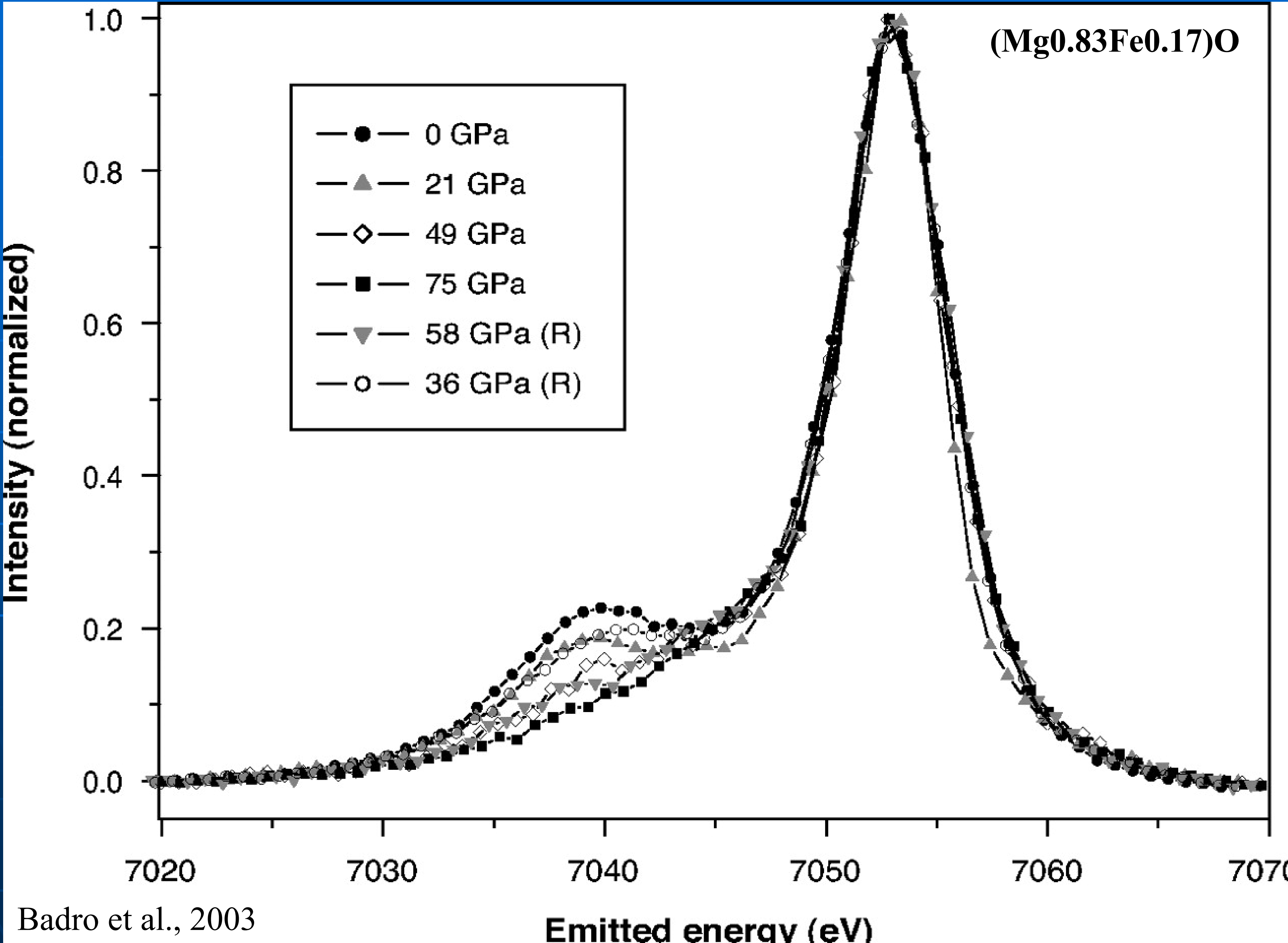
Elastic moduli, thermal conductivity, electrical transport, and other physical and chemical properties of Fe-bearing minerals could thus be dramatically changed at depth due to the spin transition. Consequently, there has been much interest in the spin transition, and high-pressure studies have demonstrated that it can indeed take place in the minerals present in the deep mantle.


α
β
γ
gt
opx + cpx
mw
pv
cpv
stish
CaCl2
wust
rhomb
corun
Rh2O3(II)
Depth (km)
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
P (GPa)
29.2
38.2
47.5
56.9
66.5
76.4
86.5
96.8
107.4
118.4
129.8
0
20
40
60
80
100
Volume Fraction (%)
0.0
0.5
1.0
1.5
K pv-mw Mg-Fe

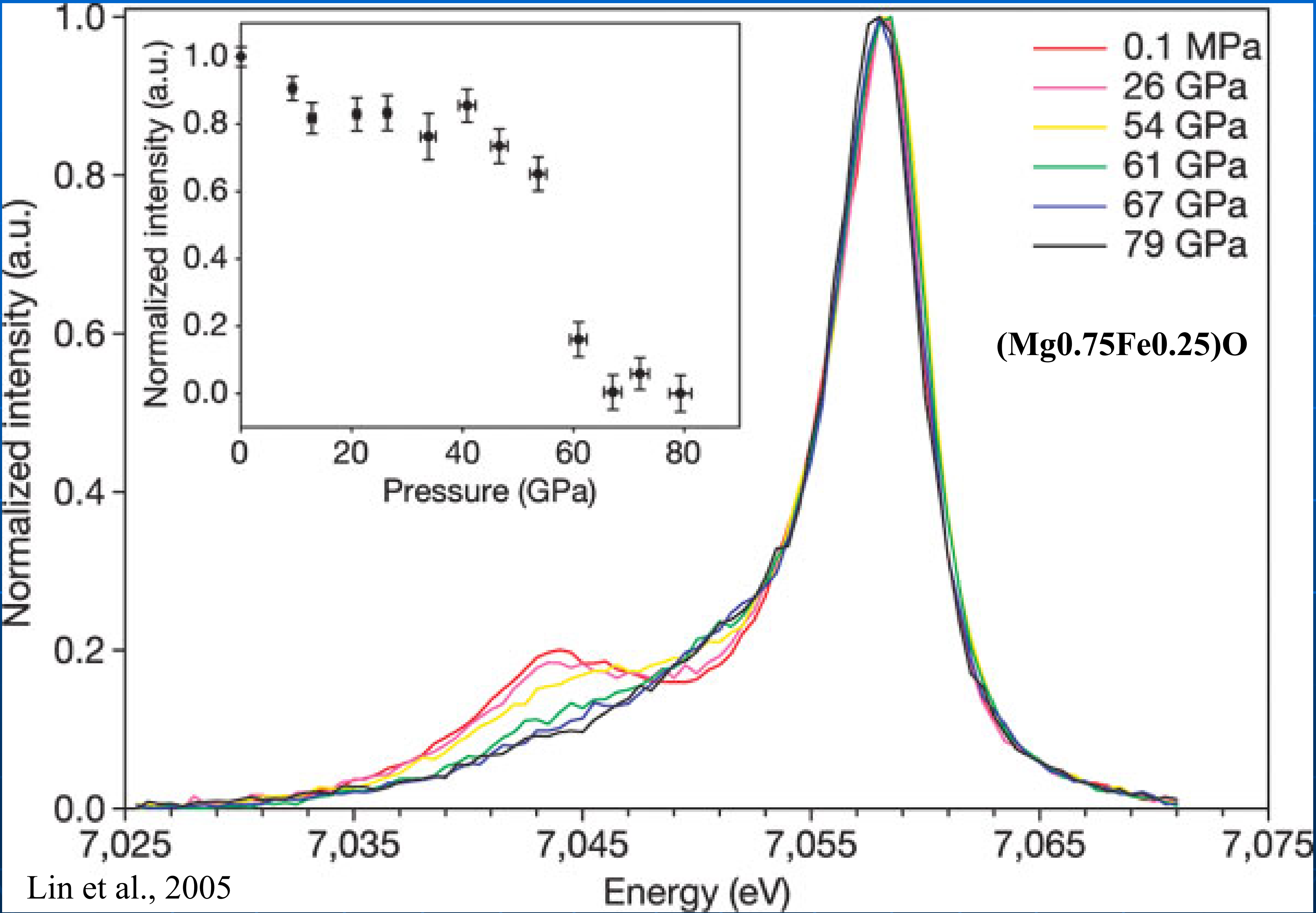
Bina, 1998



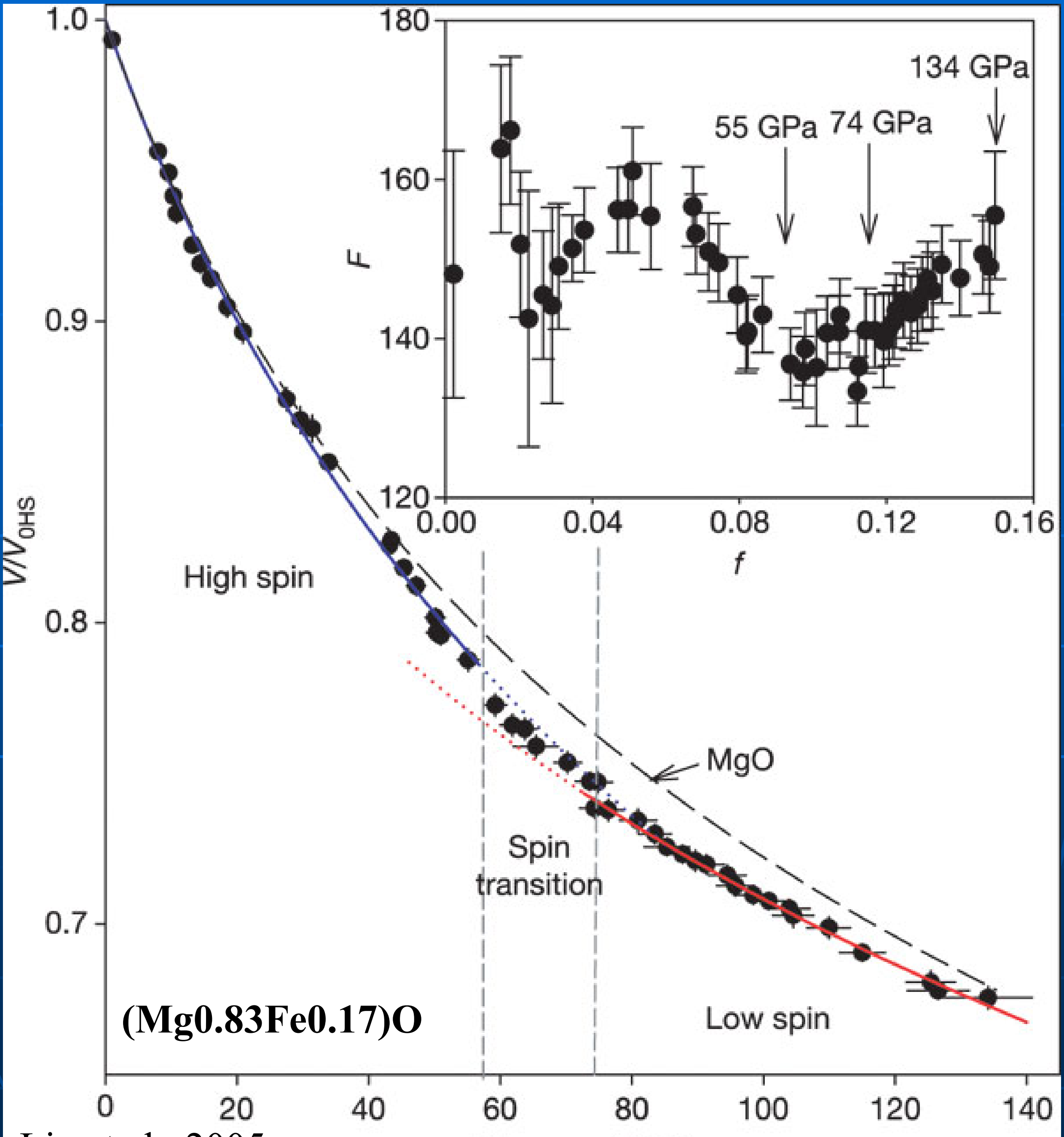
Speziale et al., 2005



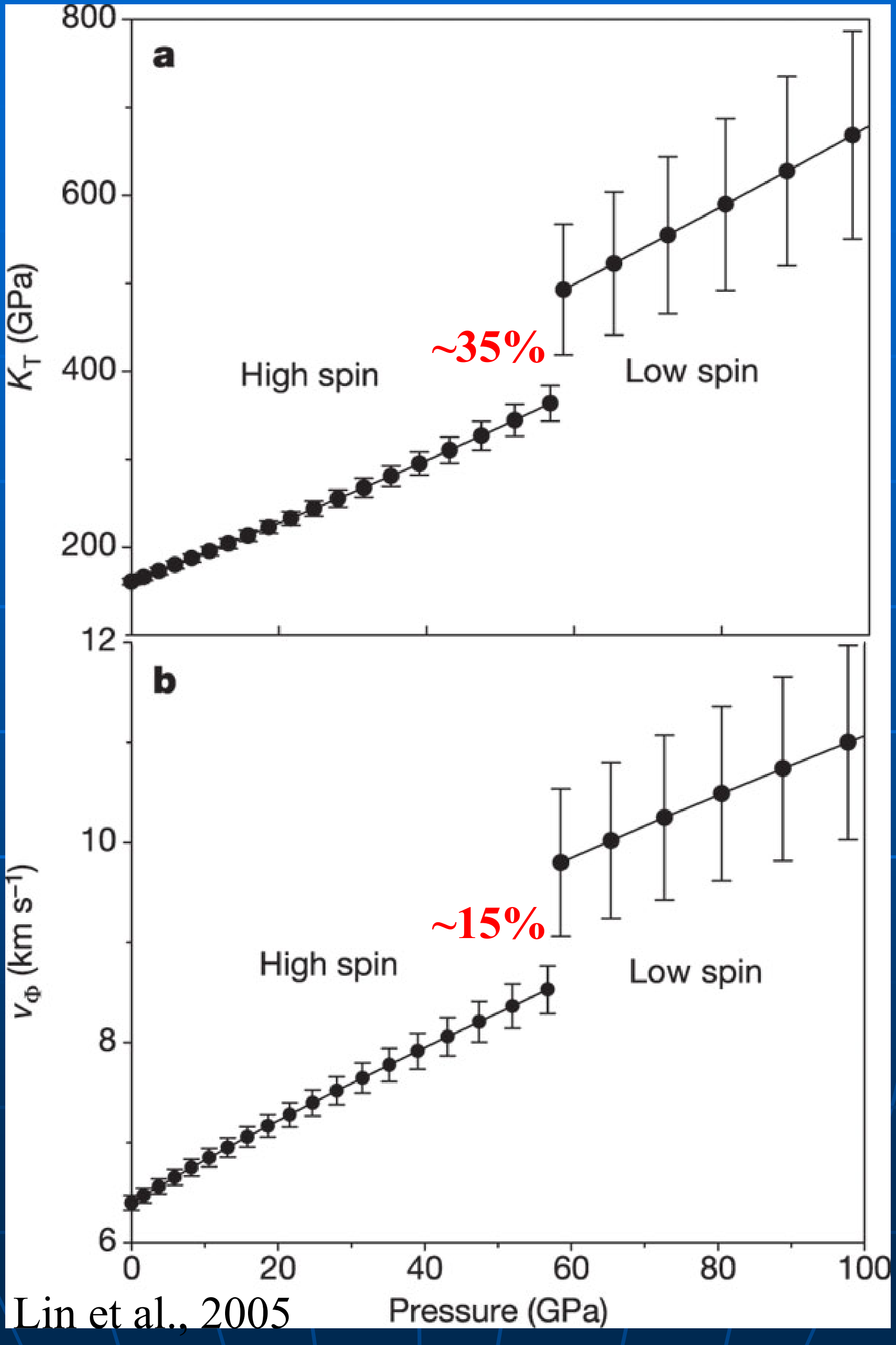
Badro et al., 2003



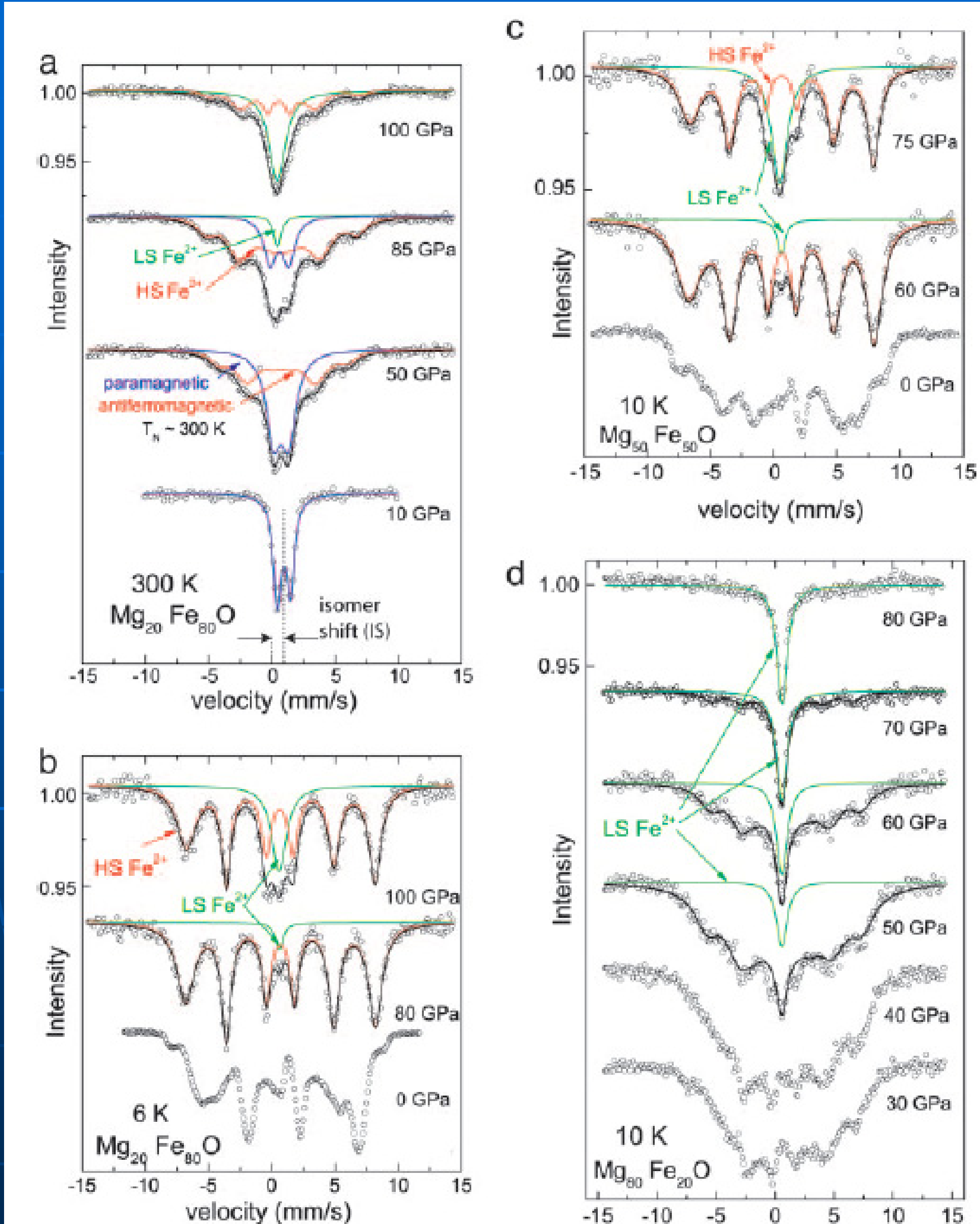
Lin et al., 2005



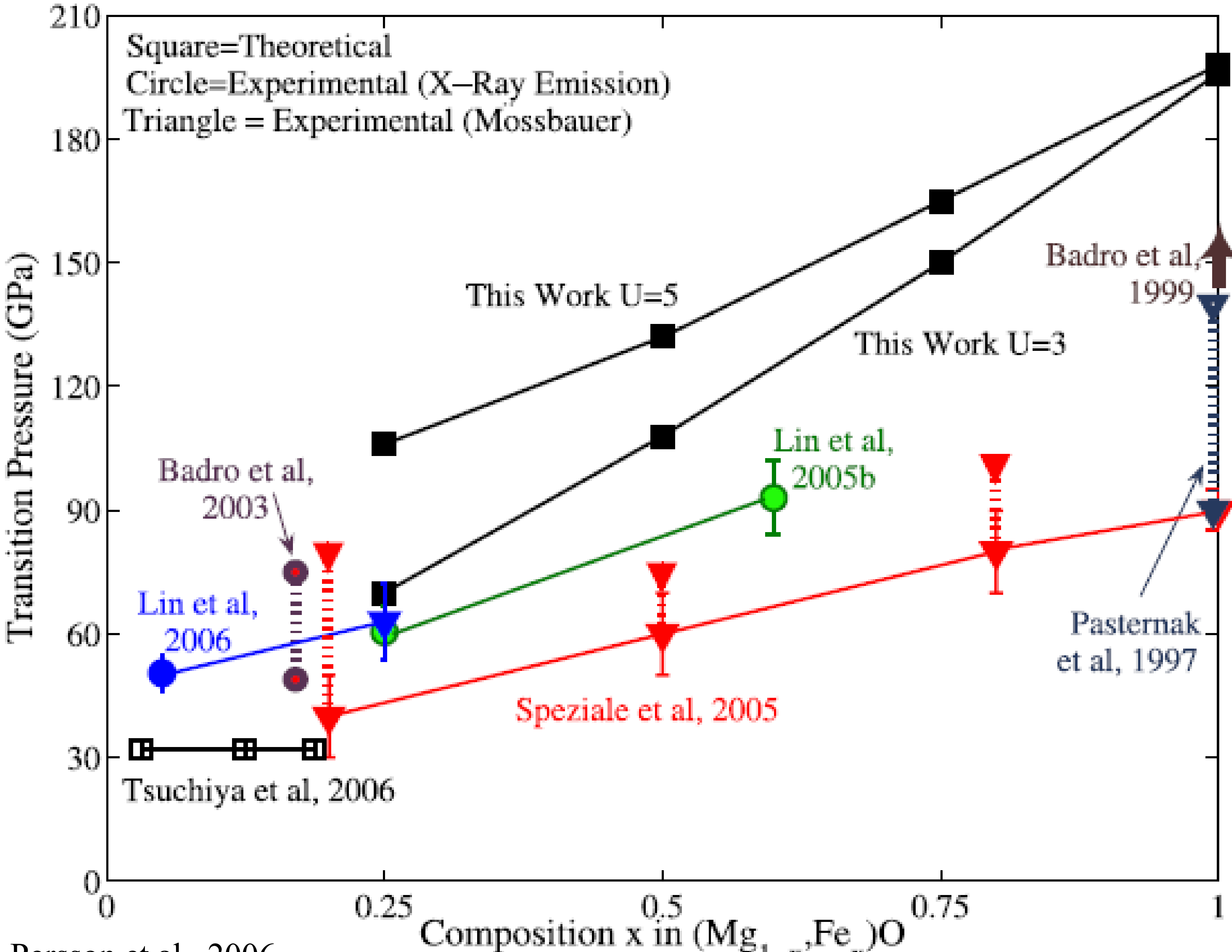
Lin et al., 2005



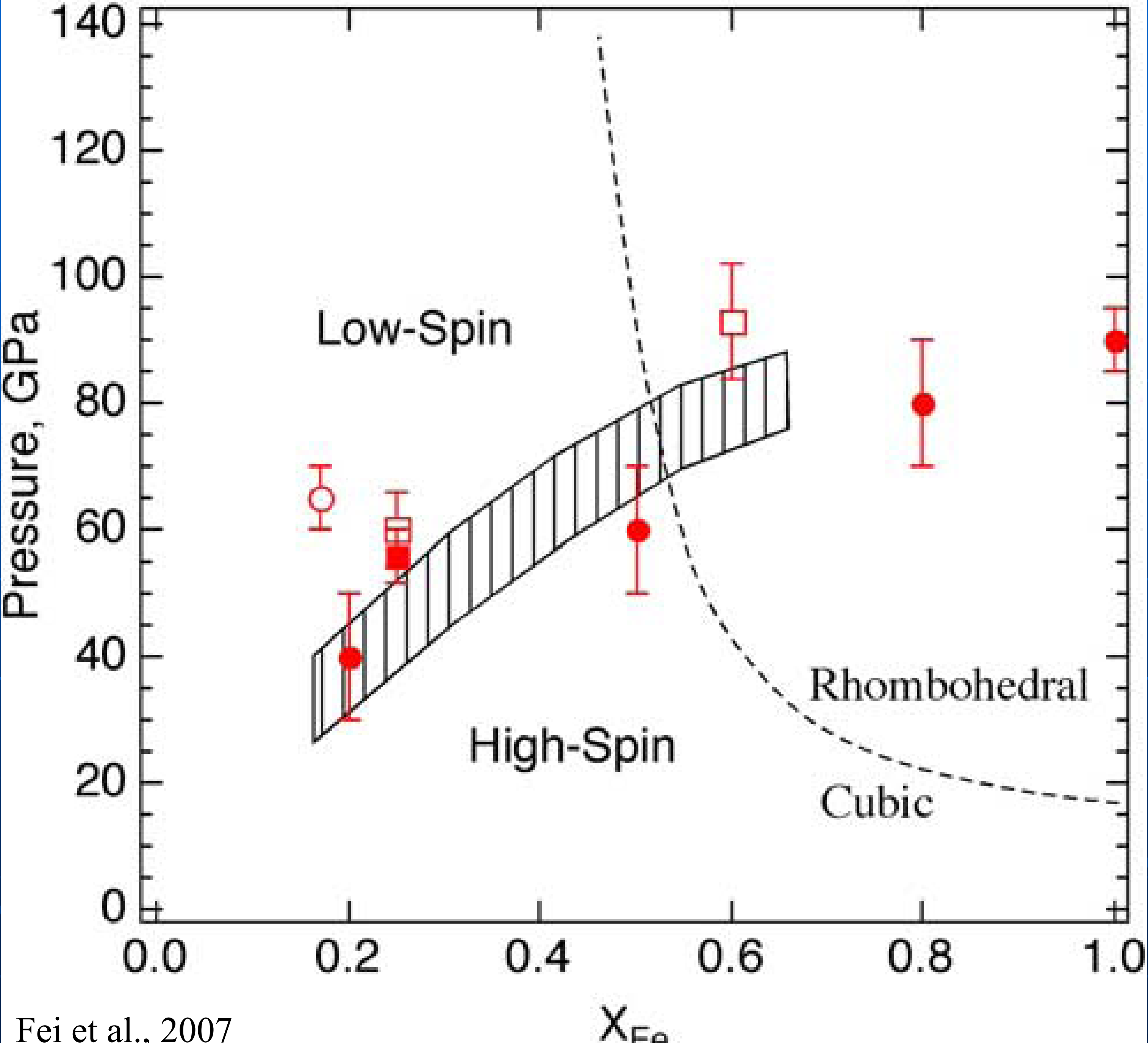
Lin et al., 2005



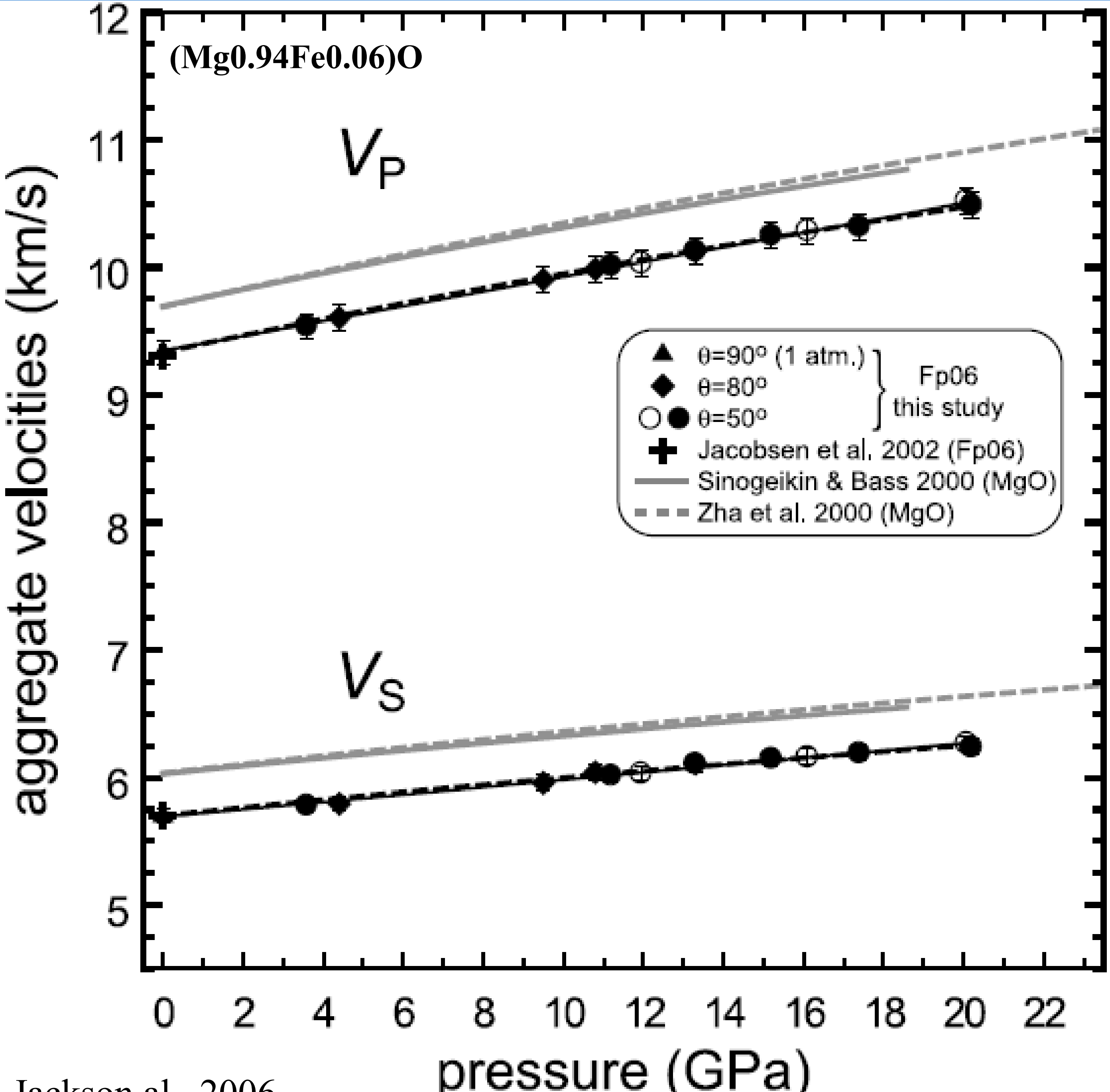
Speziale et al., 2005



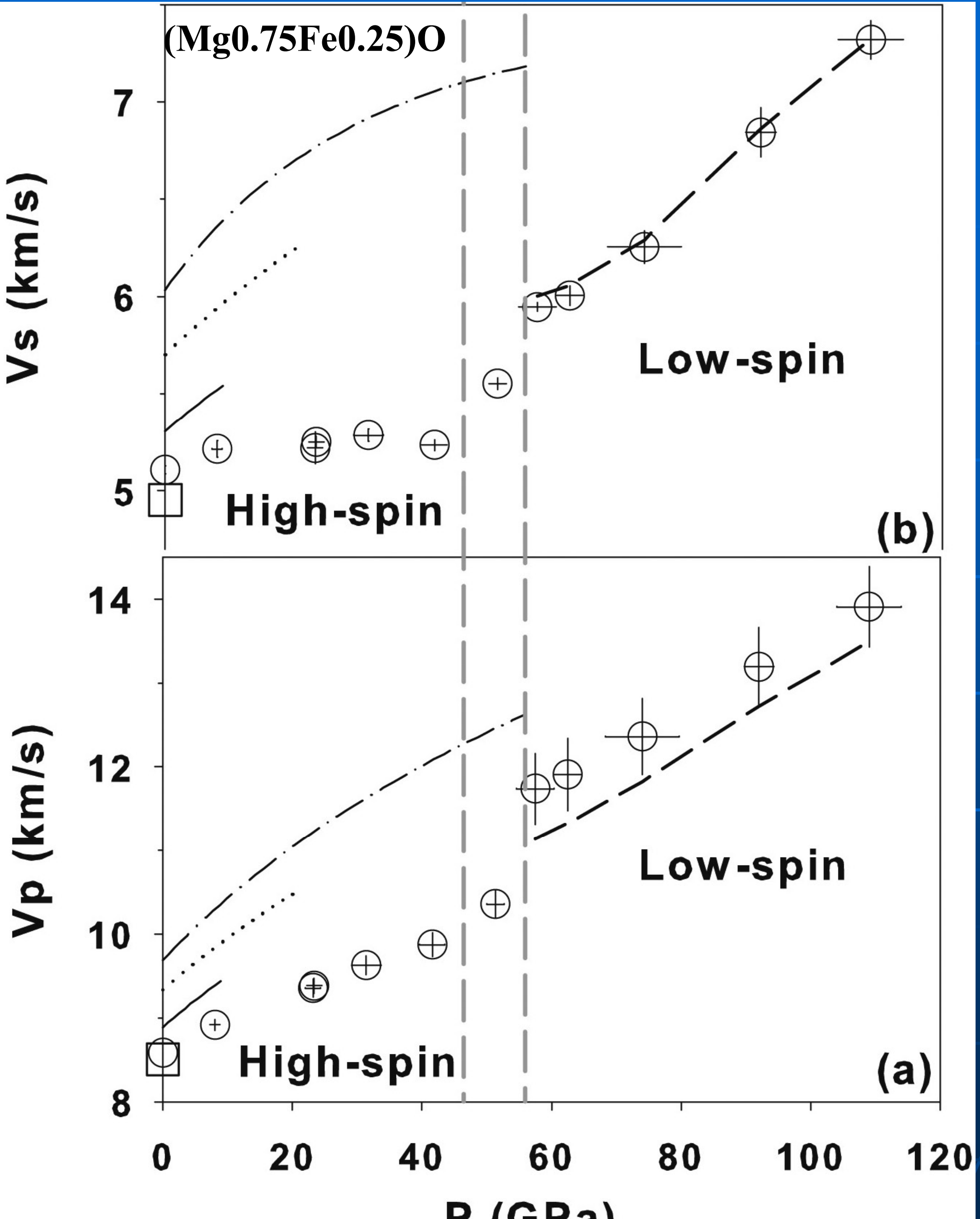
Persson et al., 2006



Fei et al., 2007



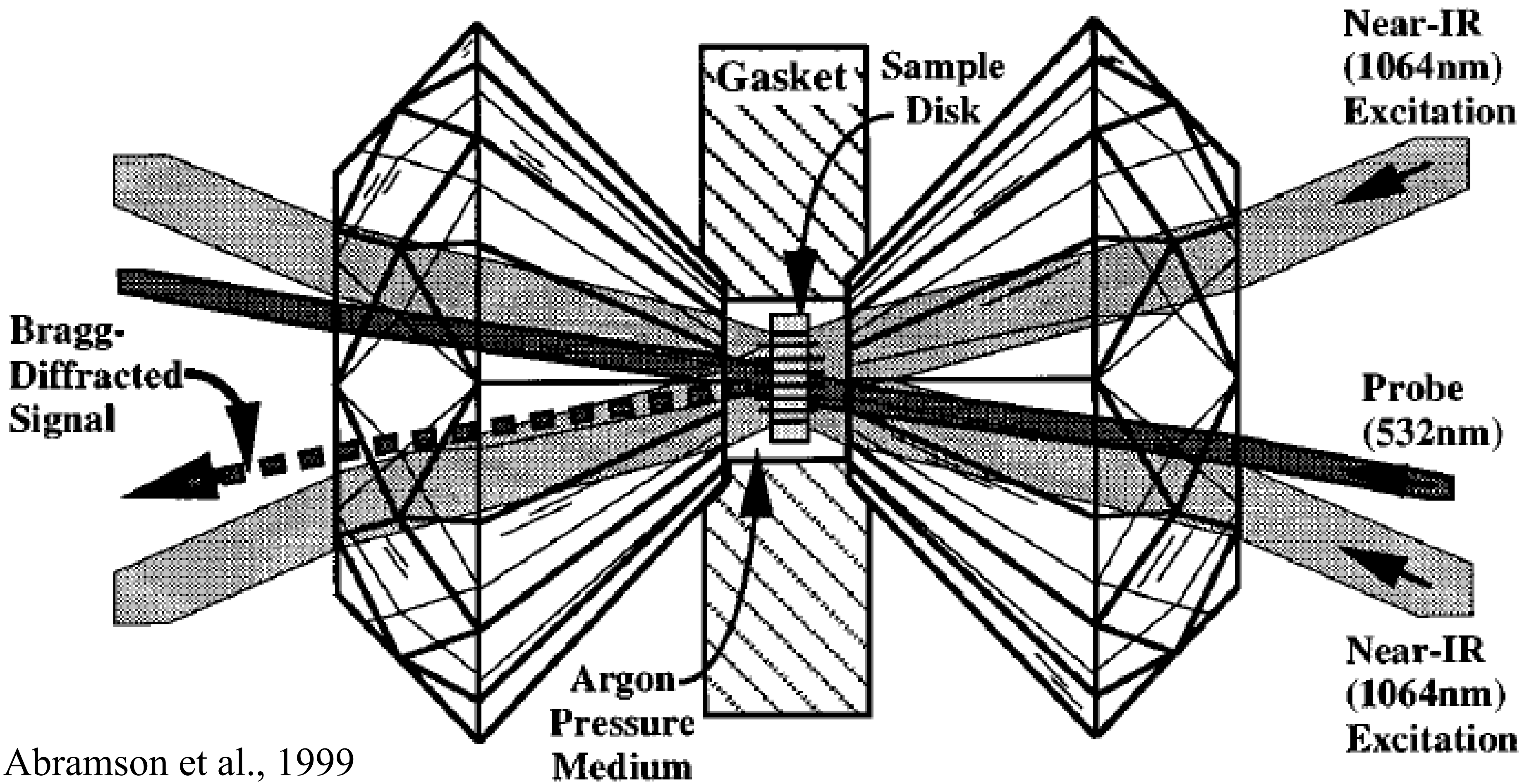
Jackson al., 2006



Lin et al., 2006

Material: $(Mg_{0.944},Fe_{0.056})O$ single crystals (55×45 ×15 μm)

Method: DAC + ISLS (Impulsive Stimulated Light Scattering)



Abramson et al., 1999

Table S1. Acoustic velocities for propagation in the (100)-type plane of $(Mg_{0.944},Fe_{0.056})O$ in argon as a function of pressure, *P*. Compressional velocities (V_p) have uncertainties of 0.5% and are reported in two crystallographic directions. The interfacial wave velocities have uncertainties of 1% and were found to independent of direction within the uncertainties.

P (GPa)	V_p [100] (km/s)	V_p [110] (km/s)	Interfacial (km/s)
32.5	11.22	10.94	5.52
34.0	11.44	11.03	5.63
37.7	11.58	11.16	5.66
42.0	11.71	11.17	5.66
45.6	11.67	11.05	5.63
49.3	11.65	10.78	5.69
52.7	12.03	11.16	5.80
56.5	12.67	11.67	6.03
58.4	12.80	11.85	6.14
63.0	13.05		

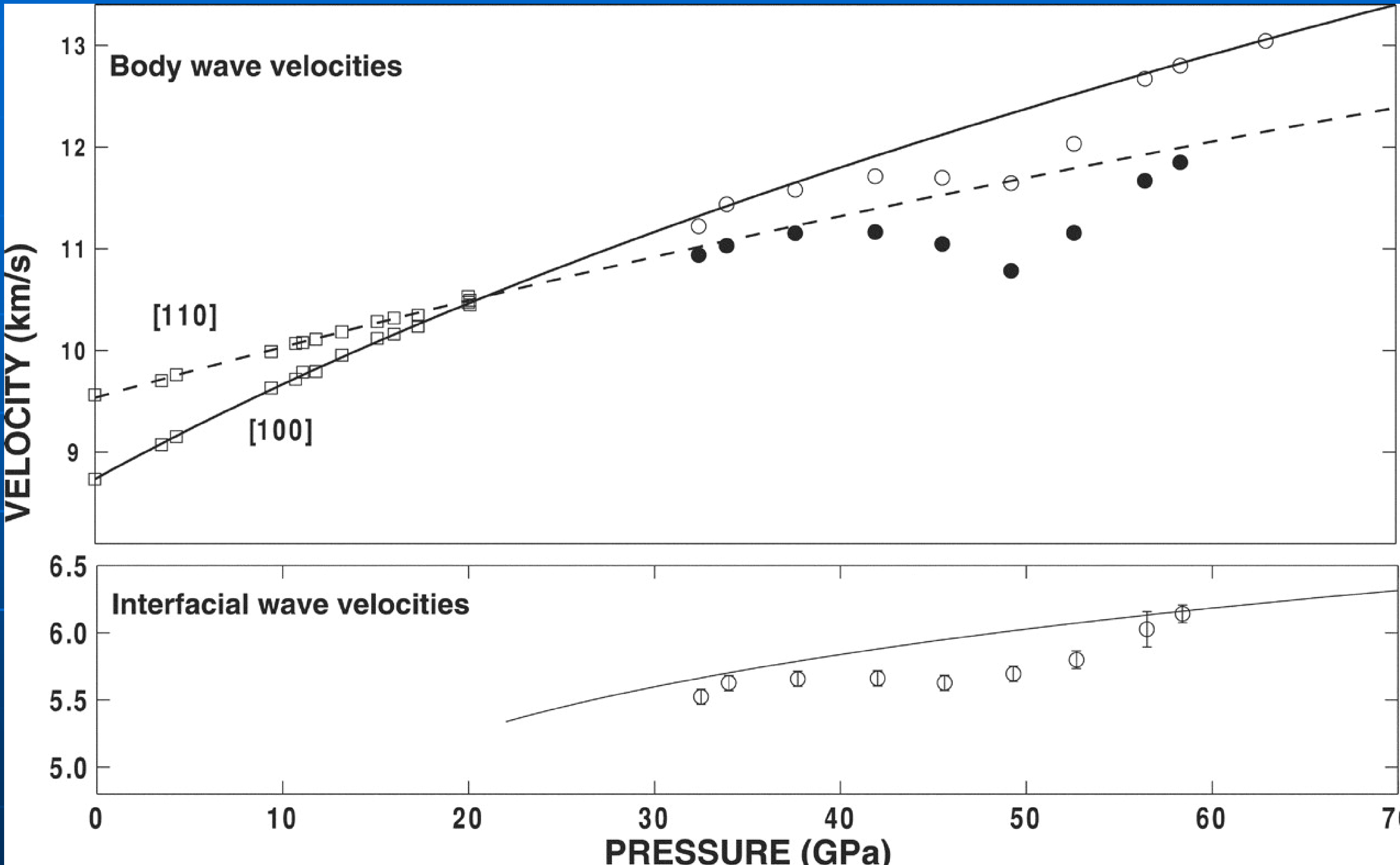
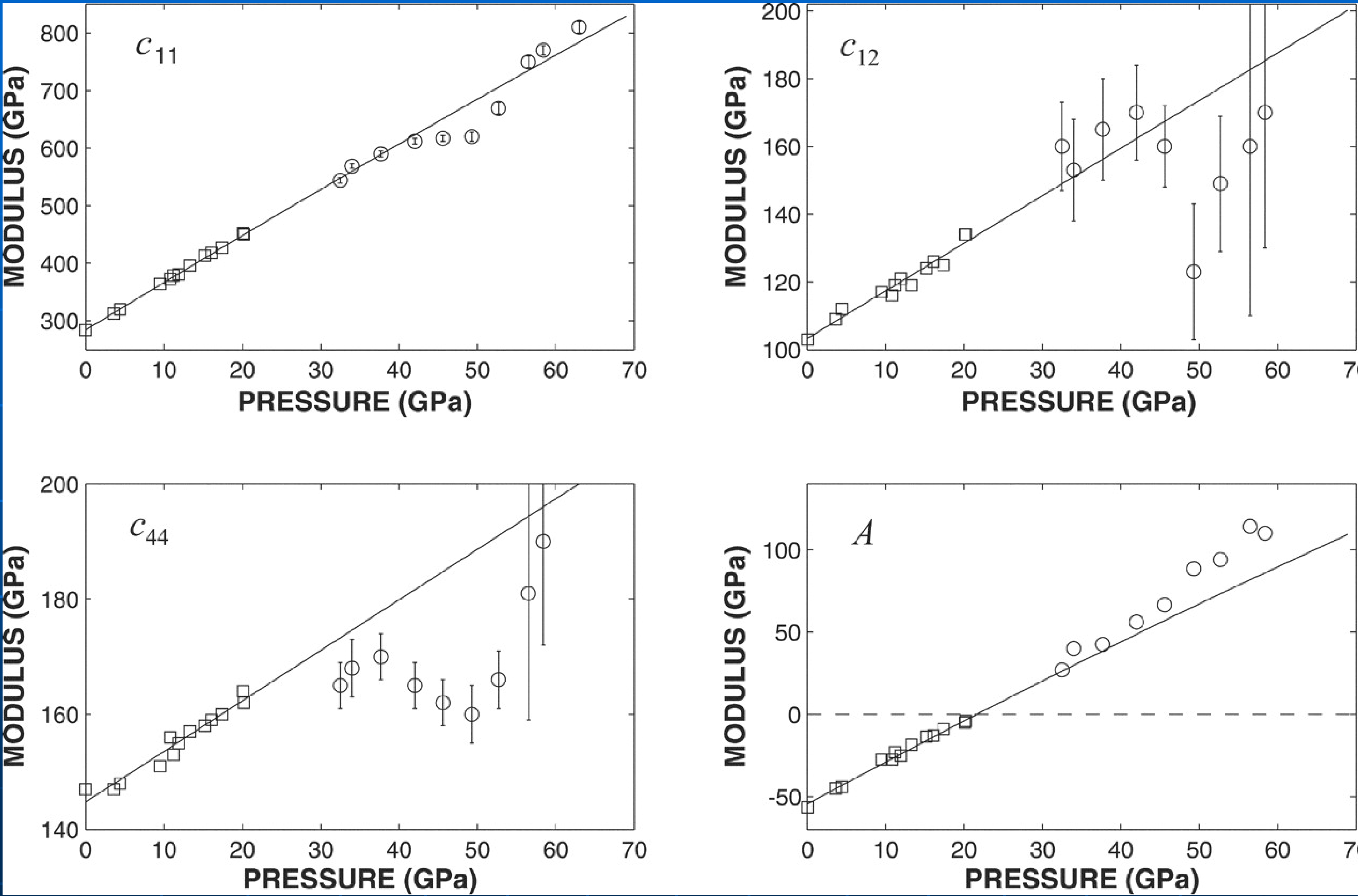
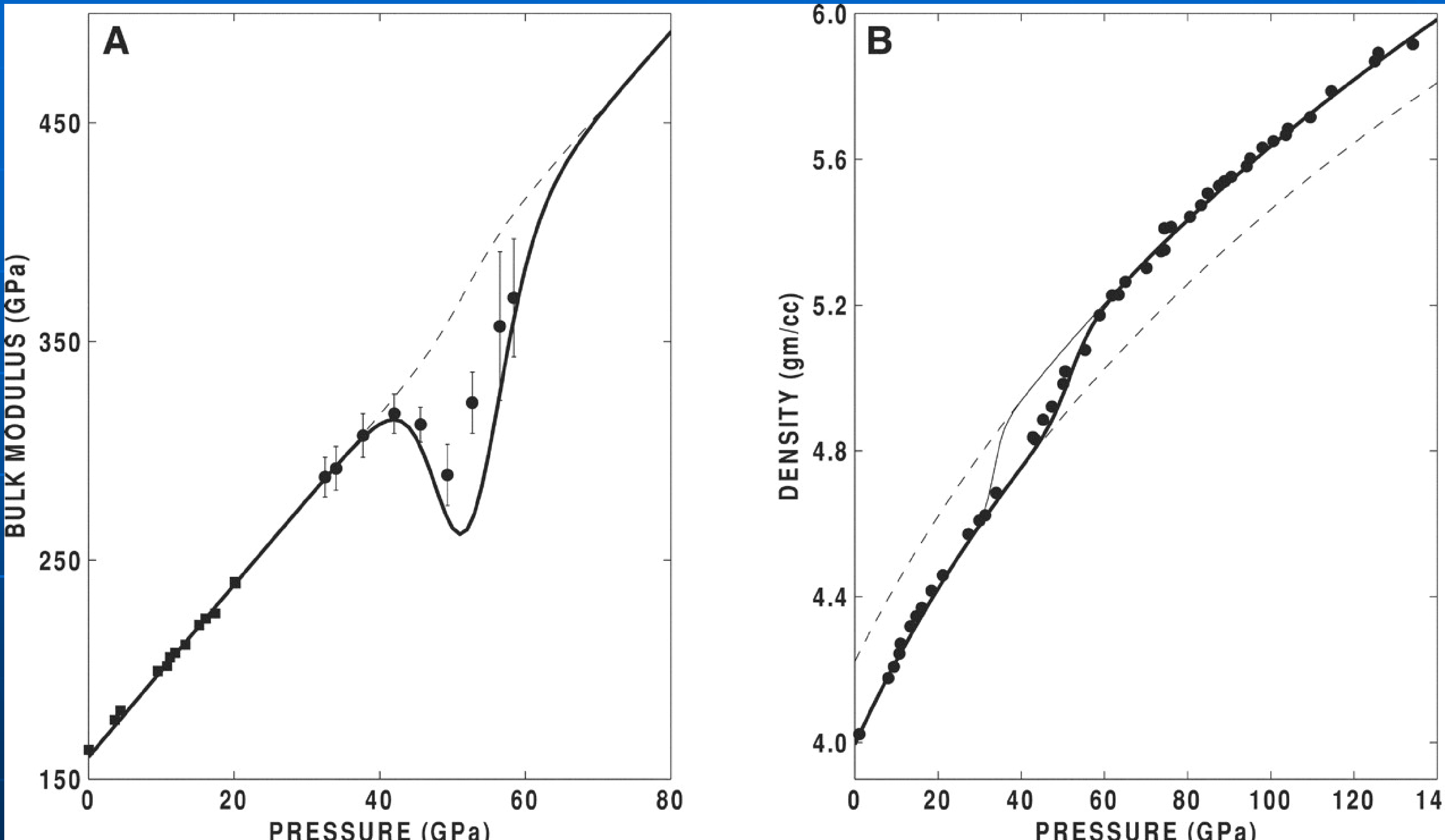

Body wave velocities
[110]
[100]
Interfacial wave velocities
VELOCITY (km/s)
PRESSURE (GPa)
13
12
11
10
9
6.5
6.0
5.5
5.0
0
10
20
30
40
50
60
70

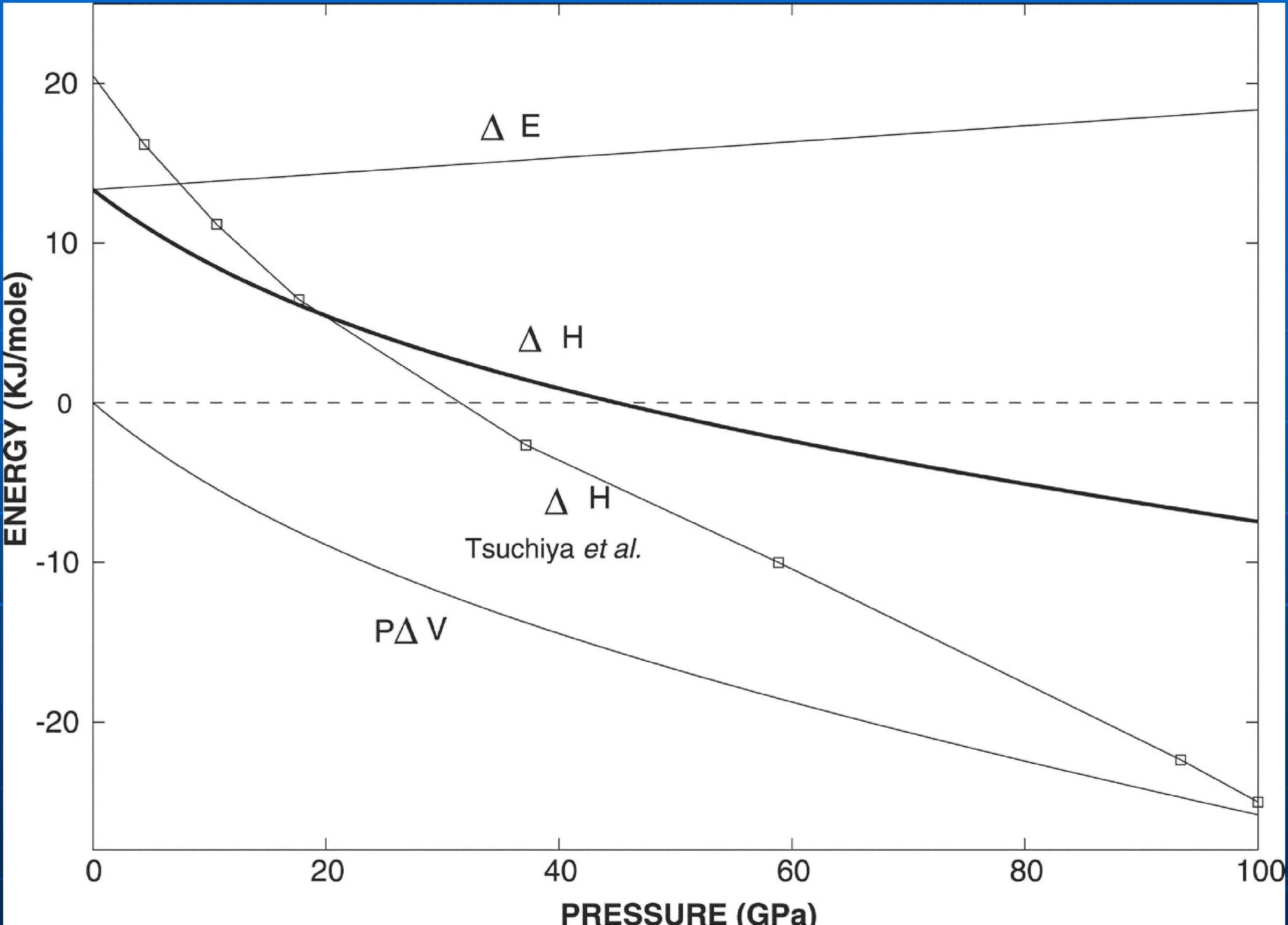
Table S2. Derived elastic moduli, c_{ij}, density, ρ, bulk modulus, K, and shear modulus G, at the indicated pressures, P for $(Mg_{0.944},Fe_{0.056})O$. Densities were recursively determined by integration of the bulk modulus. The shear modulus is the average of the Voigt and Reuss estimates obtained from the c_{ij}. Reported uncertainties are 2σ values based on fits to the velocities.

P (GPa)	ρ (gm/cc)	c_{11} (GPa)	c_{12} (GPa)	c_{44} (GPa)	K (GPa)	G (GPa)
32.5	4.32	544(5)	160(13)	165(4)	288(9)	175(4)
34.0	4.35	569(4)	153(15)	168(5)	292(10)	182(5)
37.7	4.40	590(5)	165(15)	170(4)	307(10)	185(4)
42.0	4.46	612(5)	170(14)	165(4)	317(9)	184(4)
45.6	4.51	617(5)	160(12)	162(4)	312(8)	183(4)
49.3	4.57	620(8)	123(20)	160(5)	289(14)	187(5)
52.7	4.62	669(10)	149(20)	166(5)	322(14)	194(5)
56.5	4.67	750(10)	160(50)	181(22)	357(34)	214(17)
58.4	4.70	770(8)	170(40)	190(18)	370(27)	223(14)
63.0	4.76	810(10)				


c_{11}
c_{12}
c_{44}
A
MODULUS (GPa)
PRESSURE (GPa)
800
700
600
500
400
300
200
180
160
140
120
100
50
0
-50
0
10
20
30
40
50
60
70



A
BULK MODULUS (GPa)
450
350
250
150
0
20
40
60
80
PRESSURE (GPa)
B
DENSITY (gm/cc)
6.0
5.6
5.2
4.8
4.4
4.0
0
20
40
60
80
100
120
140
PRESSURE (GPa)



ENERGY (KJ/mole)
20
10
0
-10
-20
0
20
40
60
80
100
PRESSURE (GPa)
Δ E
Δ H
Δ H
Tsuchiya et al.
PΔ V

Conclusions

1. The elastic moduli of (Mg1–x,Fex)O (x = 0.06) ferropericlase exhibited up to 25% softening over an extended pressure range from 40 to 60 GPa. The magnitude of softening increases with iron content up to at least x = 0.20.

2. The spin transition in (Mg,Fe)O is too broad to produce an abrupt seismic discontinuity in the lower mantle,and the transition will produce a correlated negative anomaly for both compressional and shear velocities that extends throughout most, if not all, of the lower mantle.