Partitioning of iron between perovskite, post-perovskite, and ferropericlase up to 154 GPa and 2000 K

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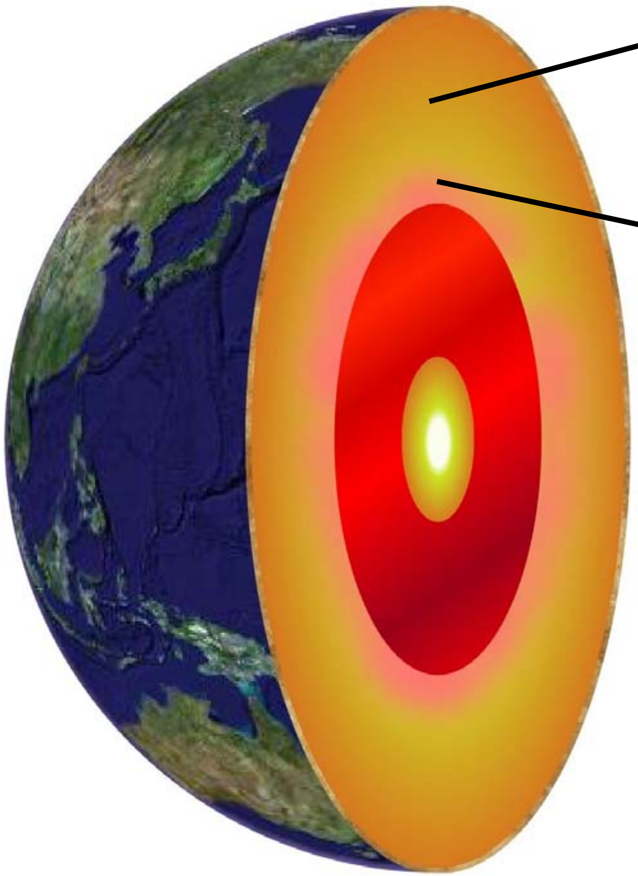
SPring-8

Introduction



(Mg,Fe)SiO$_3$ Perovskite (Pv)
(Mg,Fe)O Ferropericlase(Fp)

Post-Pv phase
Fp

Partition coefficient (K) of Fe-Mg between Pv/PPv and Fp

$$K = \left(\frac{X_{Fe}}{X_{Mg}}\right)^{Pv\ or\ PPv} \Big/ \left(\frac{X_{Fe}}{X_{Mg}}\right)^{Fp}$$

$$X_{Fe} = FeO/(FeO + MgO)$$

in molar ratio

Fe-Mg partitioning between these phases is important for understanding the chemical and physical properties (e.g. density, elastic velocity) of Earth's lower mantle.

Partition coefficient (K) of Fe-Mg between Pv and Fp

Pressure dependency of *K* between Pv and Fp

K increases with pressure

Mao et al., 1997
Andrault, 2001; K>1 above 70-80GPa

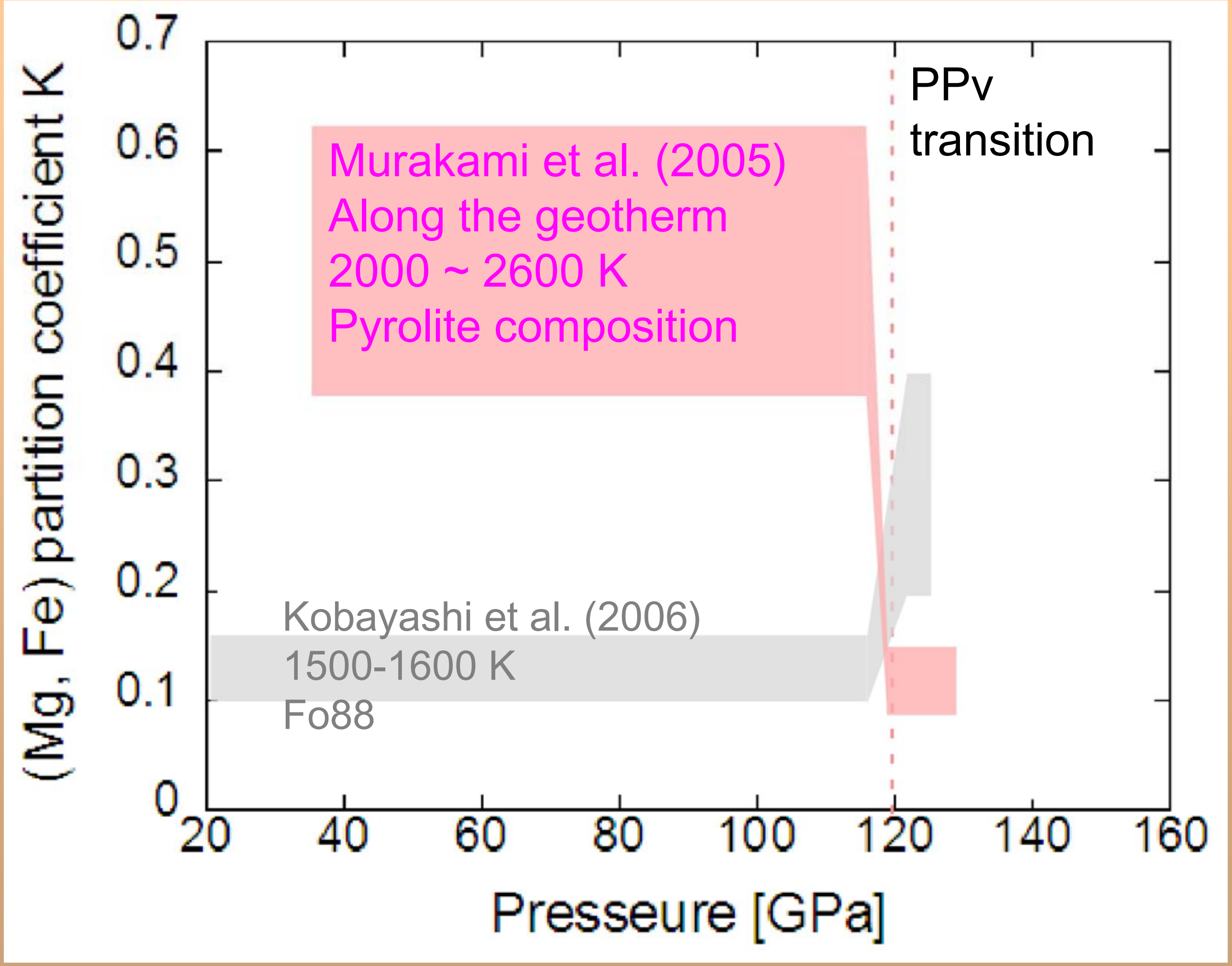
Determined by X-ray (unit cell volume)

K is almost constant with pressure

Guyot et al., 1988; constant above 40GPa
Kesson et al., 1991, 1998, 2002

Determined by ATEM

Partition coefficient (K) of Fe-Mg between Pv/PPv and Fp



HS-LS transition in Magnesiowüstite

Iron may strongly prefer the LS-Mw

(Badro et al., 2004)

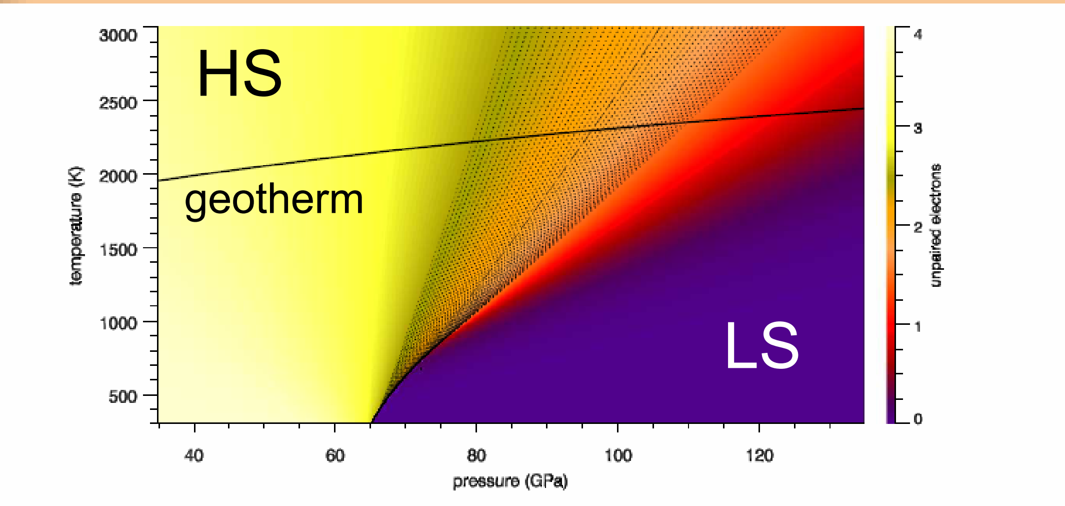
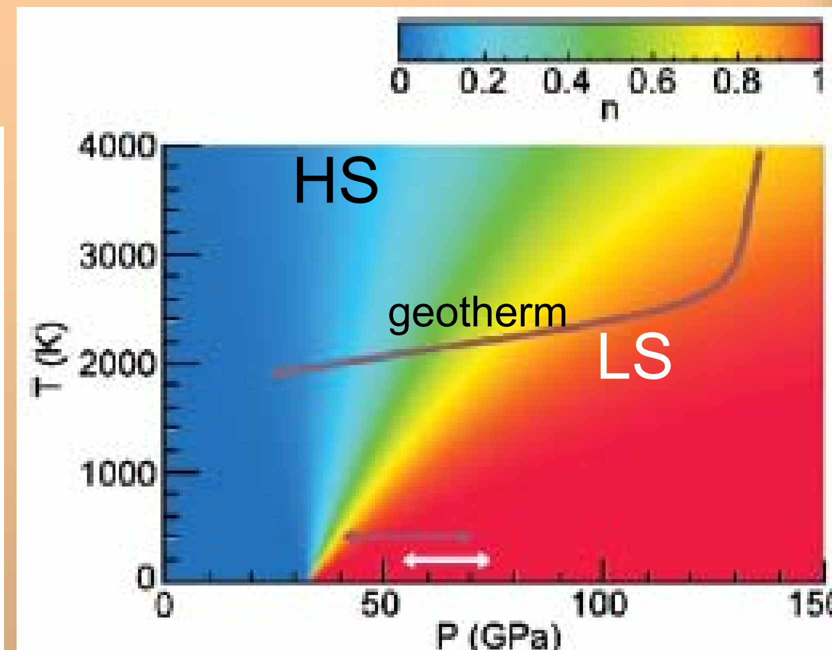


Figure 3. The average number of unpaired electrons for $Mg_{0.83}Fe_{0.17}O$ in the pressure-temperature sector. The dotted contours show the region between 1.5 and 2.5 unpaired electrons. This region clearly widens with increasing temperature. In particular, the iron spin state varies smoothly along a lower mantle geotherm [*Brown and Shankland, 1981*] given by the solid line. Parameters used for this calculation are given in the text.



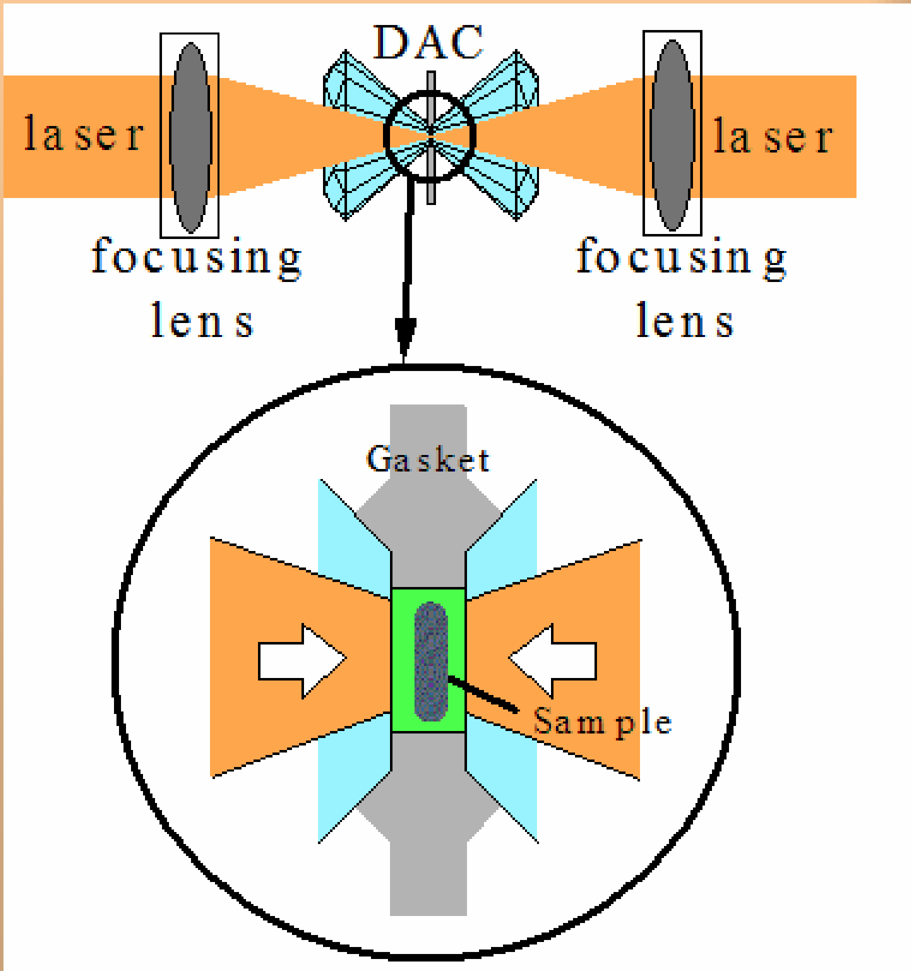
Sturhahn et al., 2005 GRL

Tsuchiya et al., 2006 PRL

Experimental procedure

Starting Material: San Carlos olivine $(Mg_{0.88}, Fe_{0.12})_2SiO_4$
Al-free system

High P-T generation: Laser-Heated diamond anvil cell
Laser spot size: ~50 μm



Pressure medium:
with or without NaCl

P measurement:
Ruby fluorescence
T2g Raman mode of Diamond
(Akahama et al., 2004)

T measurement:
Spectroradiometric method
(e.g. Boehler 2000)

Analytical methods

1. Lattice volume measurement at ambient condition (Determined by X-ray)

Pv : $V_0^{Pv} = 162.51 + 6.00X$ (Å)
Mw : $V_0^{Mw} = 74.78 + 6.65X$ (Å)
(X = FeO / (FeO + MgO) in molar ratio)

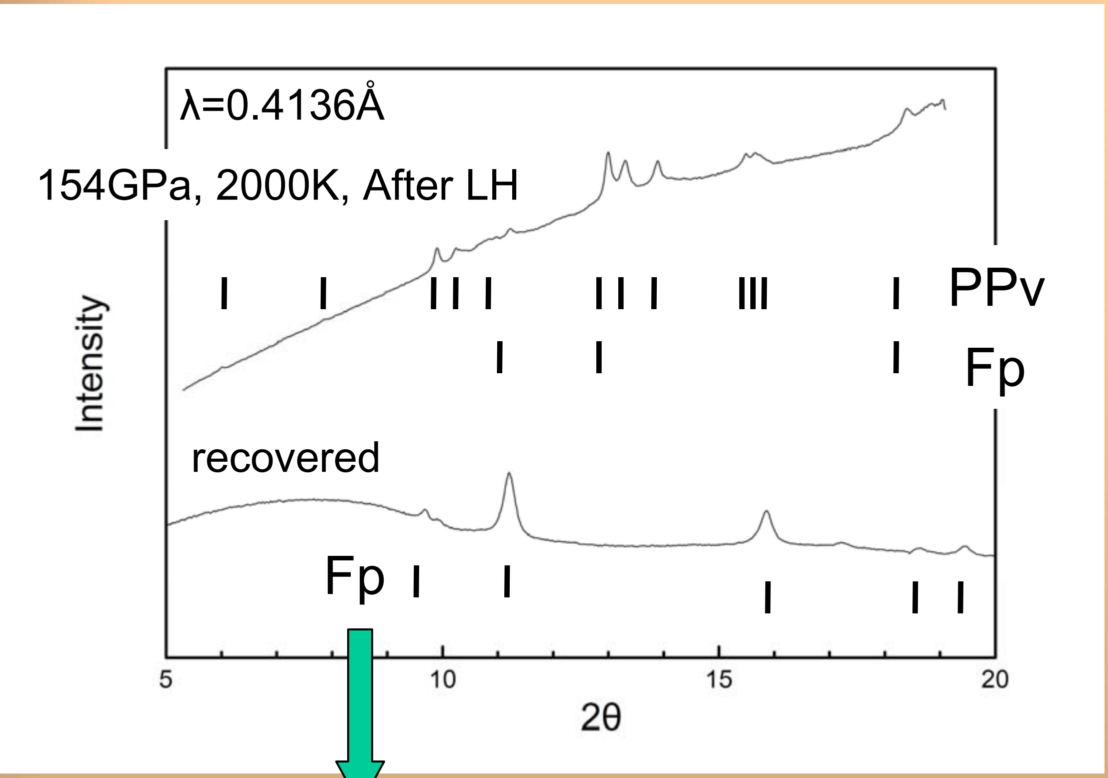
Andrault(2001)

X-ray diffraction experiments at
KEK-PF:BL-18C & SPring-8 BL10XU

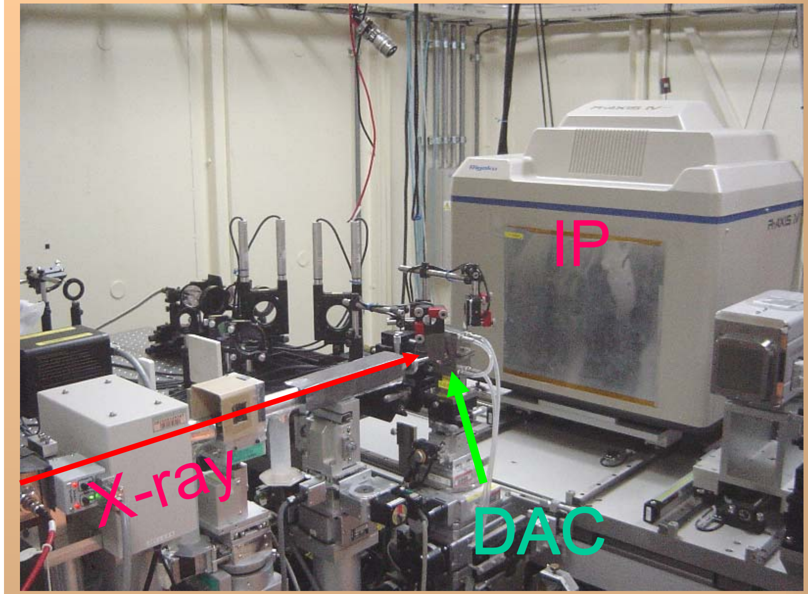
2. Analytical Transmission Electron Microscope equipped with EDS system (Determined by ATEM)

with calibrated K-factors (Cliff and Lorimer,1975; Fujino et al., 1988)
JEOL, JEM-3000F[IMR, Tohoku Univ.]

Powder X-ray diffraction



SPring-8, BL10XU



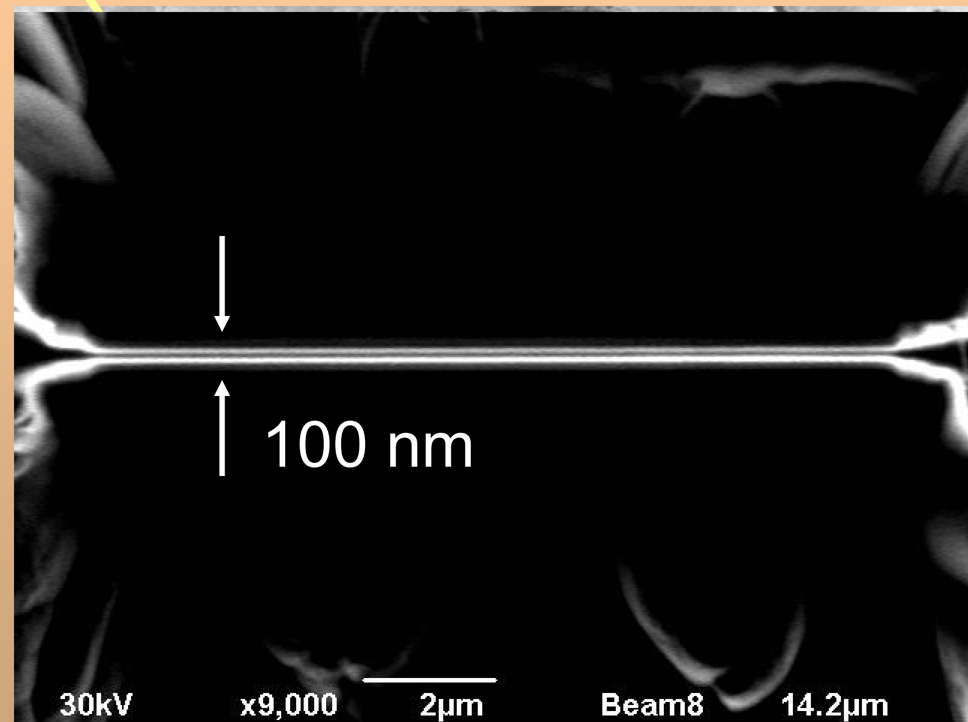
Fe#(Fp) = 0.23 (Fe# = FeO/(MgO+FeO) in the mole fraction)

Mass balance

Fe#(PPv) = 0.01

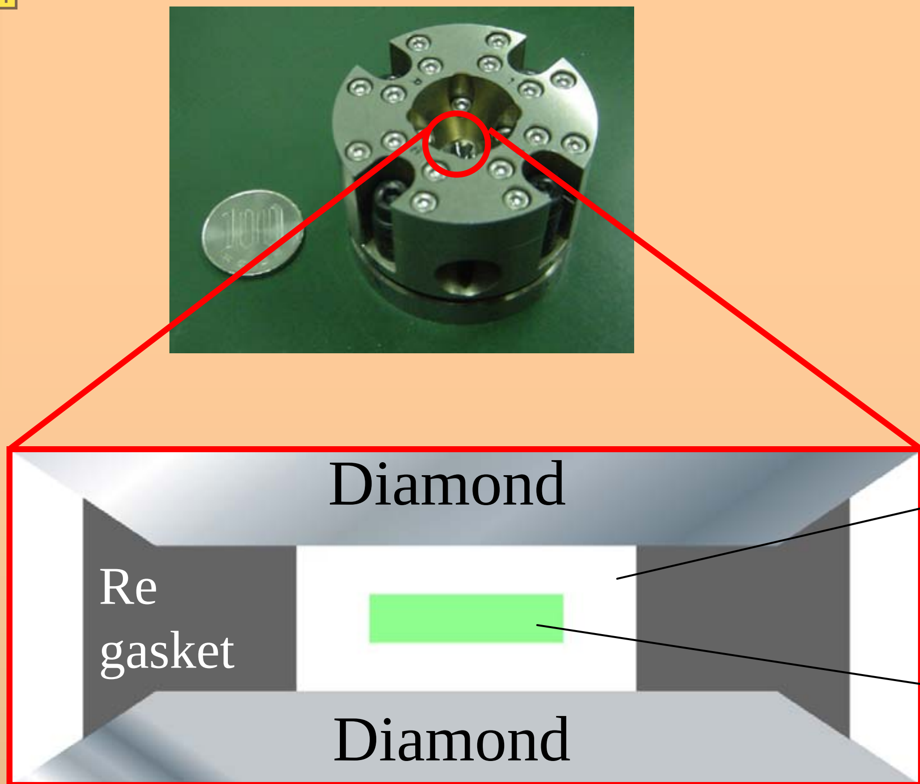
Sample preparation for TEM study by Focused Ion Beam (FIB) system

FIB system
(Tohoku univ.)



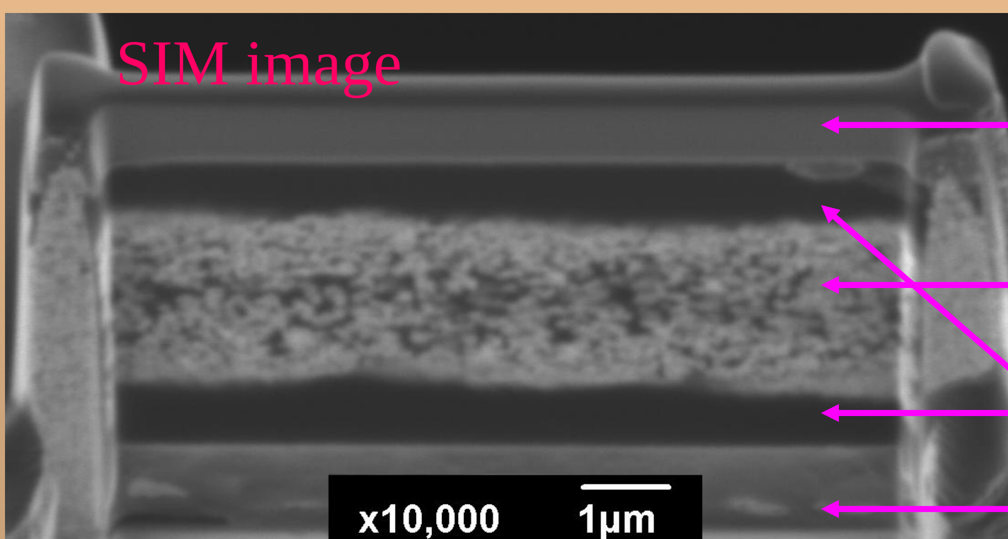
SIM image of recovered sample

Advantage of FIB



NaCl or
olivine powder

San carlos olivine
$(Mg_{0.88}, Fe_{0.12})_2SiO_4$



Carbon deposit

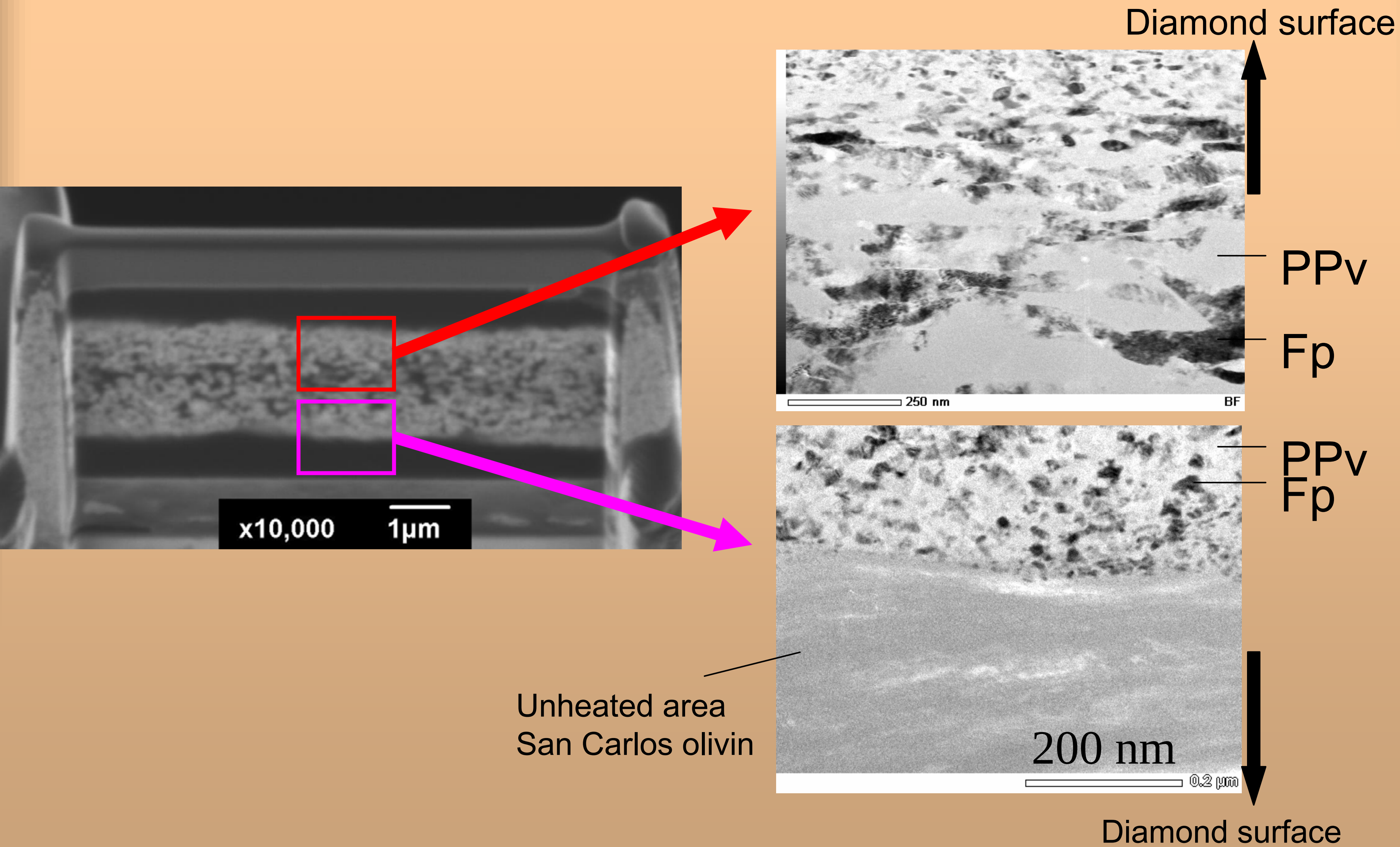
Heated area

Unheated area

Mo Grid

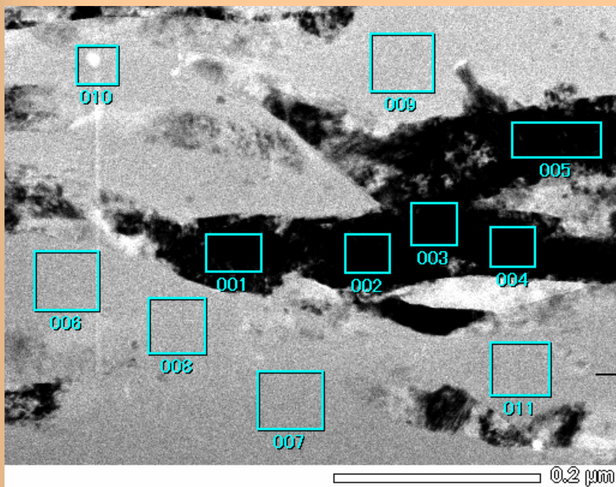
STEM image of the recovered sample

STEM image of the recovered sample from 140GPa, 2000K (90min)



Chemical analysis by ATEM

STEM image of the recovered sample from 140GPa, 2000K(90min)

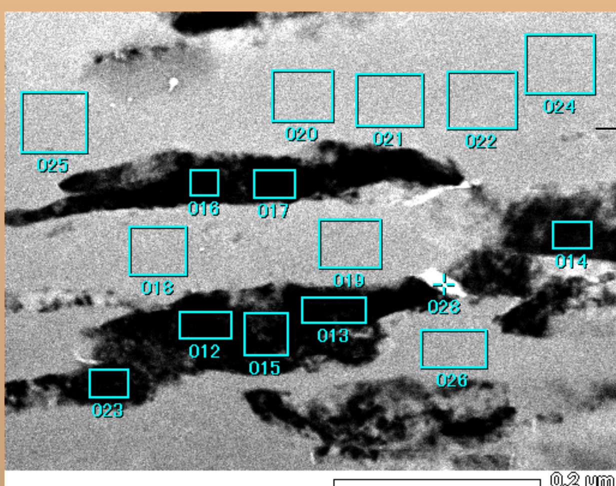


Fp

PPv

Fe#(Fp) = 0.31

Fe#(PPv) = 0.01



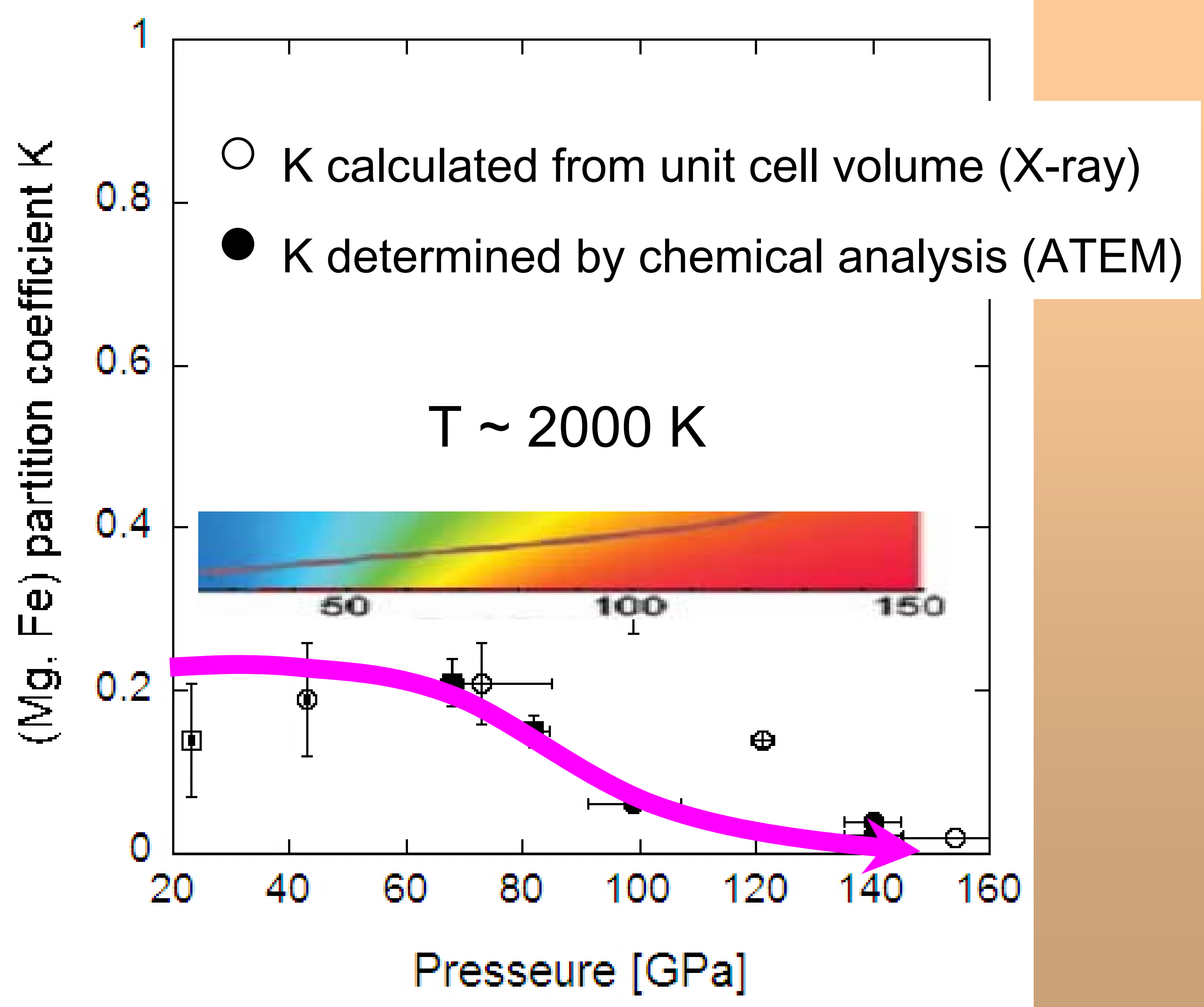
PPv

Fp

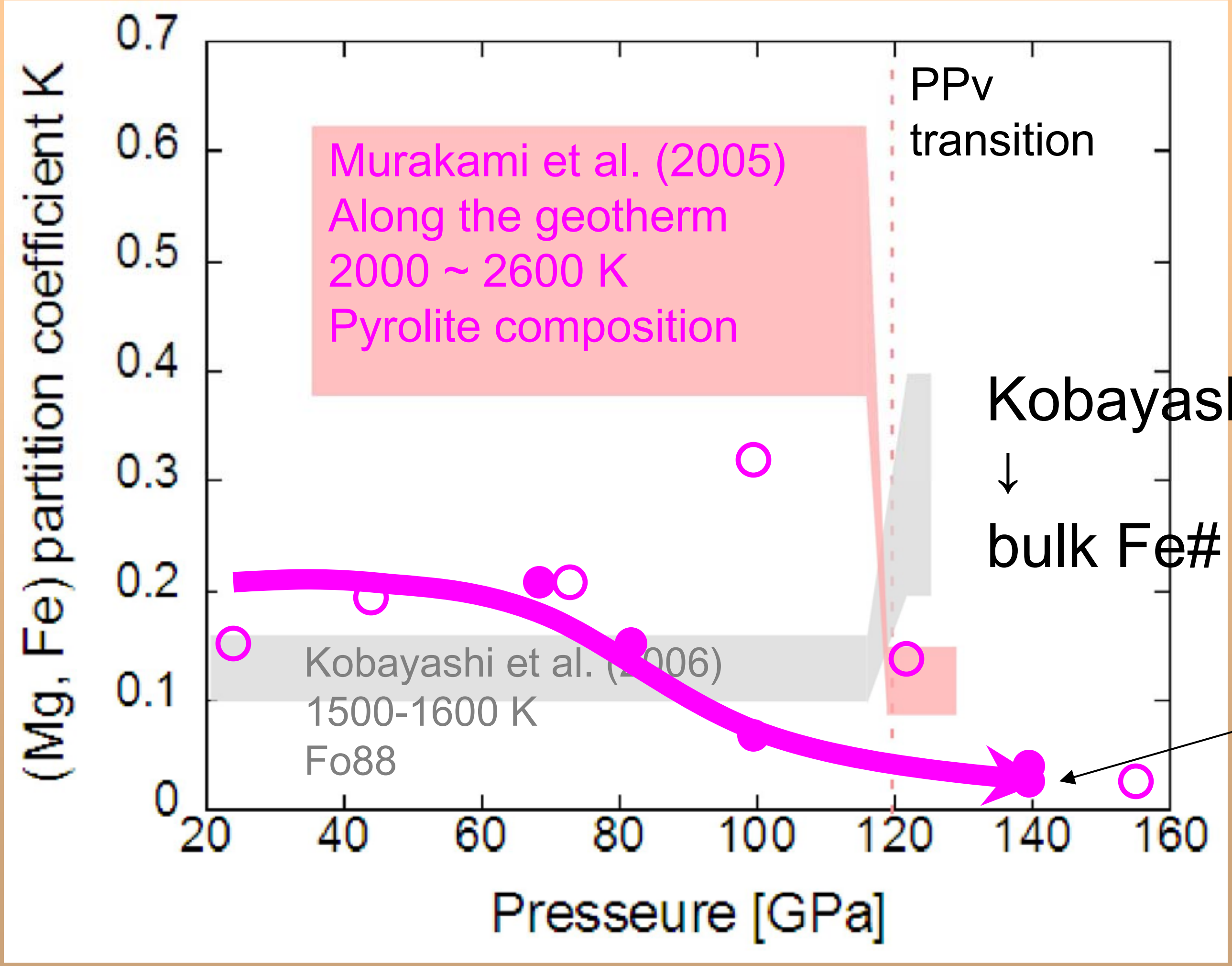
K = 0.03

200 nm

Pressure dependency of the Fe-Mg partitioning coefficient (K)



Partition coefficient (K) of Fe-Mg between Pv/PPv and Fp



Kobayashi et al.

↓

bulk Fe# reduced to 0.09

This study

↓

bulk Fe# = 0.16

Summary

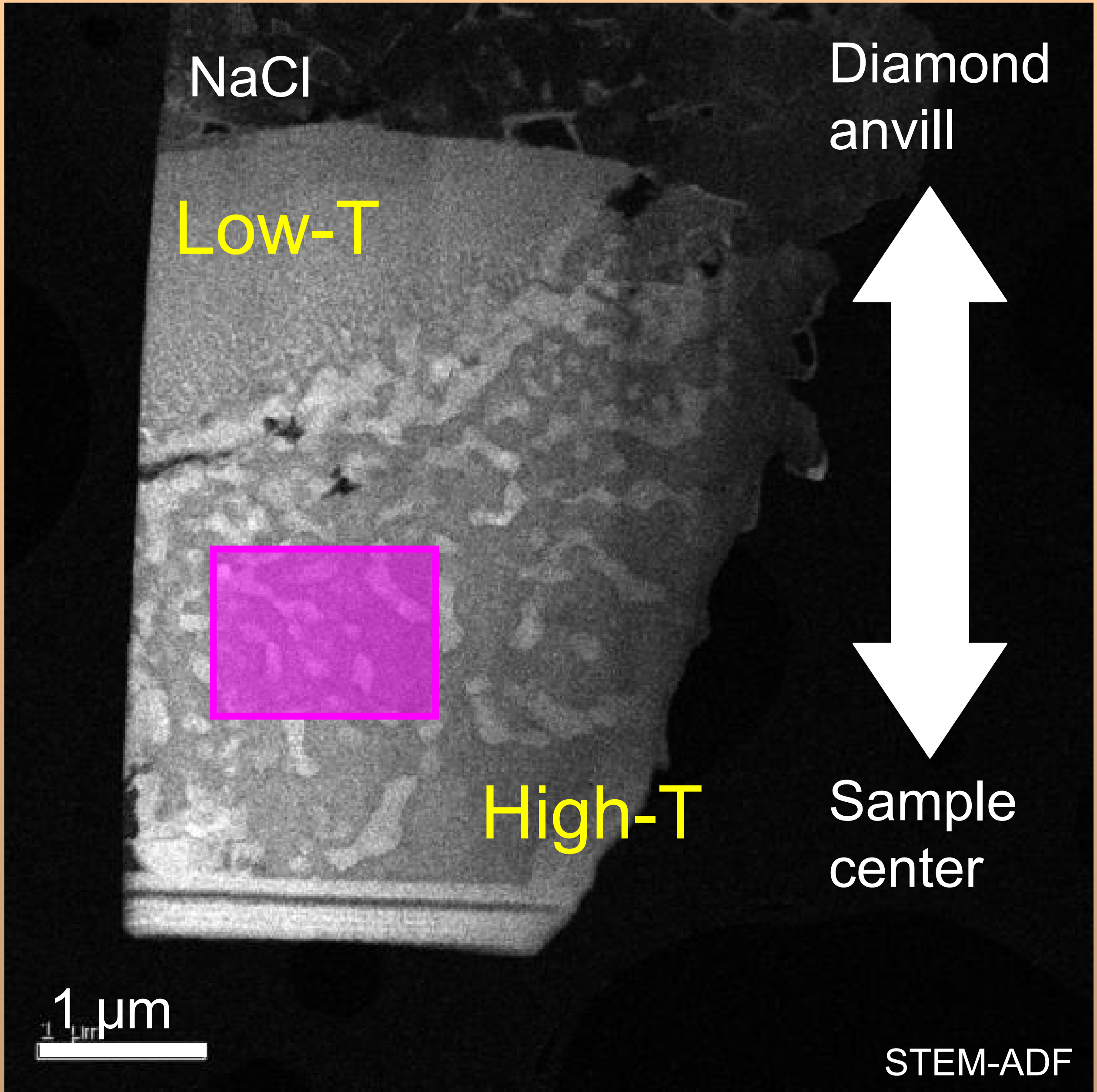
- ✓ The ATEM analysis shows that post-perovskite phase exhibits with very small iron content of Fe# = 0.01 in the recovered sample from 140 GPa and 2000 K.

- ✓ Iron prefers ferropericlase strongly rather than post-perovskite phase, which is consistent with the high-spin/low-spin transition arguments of ferropericlase [Badro et al., 2003].

- ✓ The difference in the partition coefficients between the present result and that by Kobayashi et al. (2005) may be caused by the compositional dependency of the partitioning behavior between post-perovskite and ferropericlase.

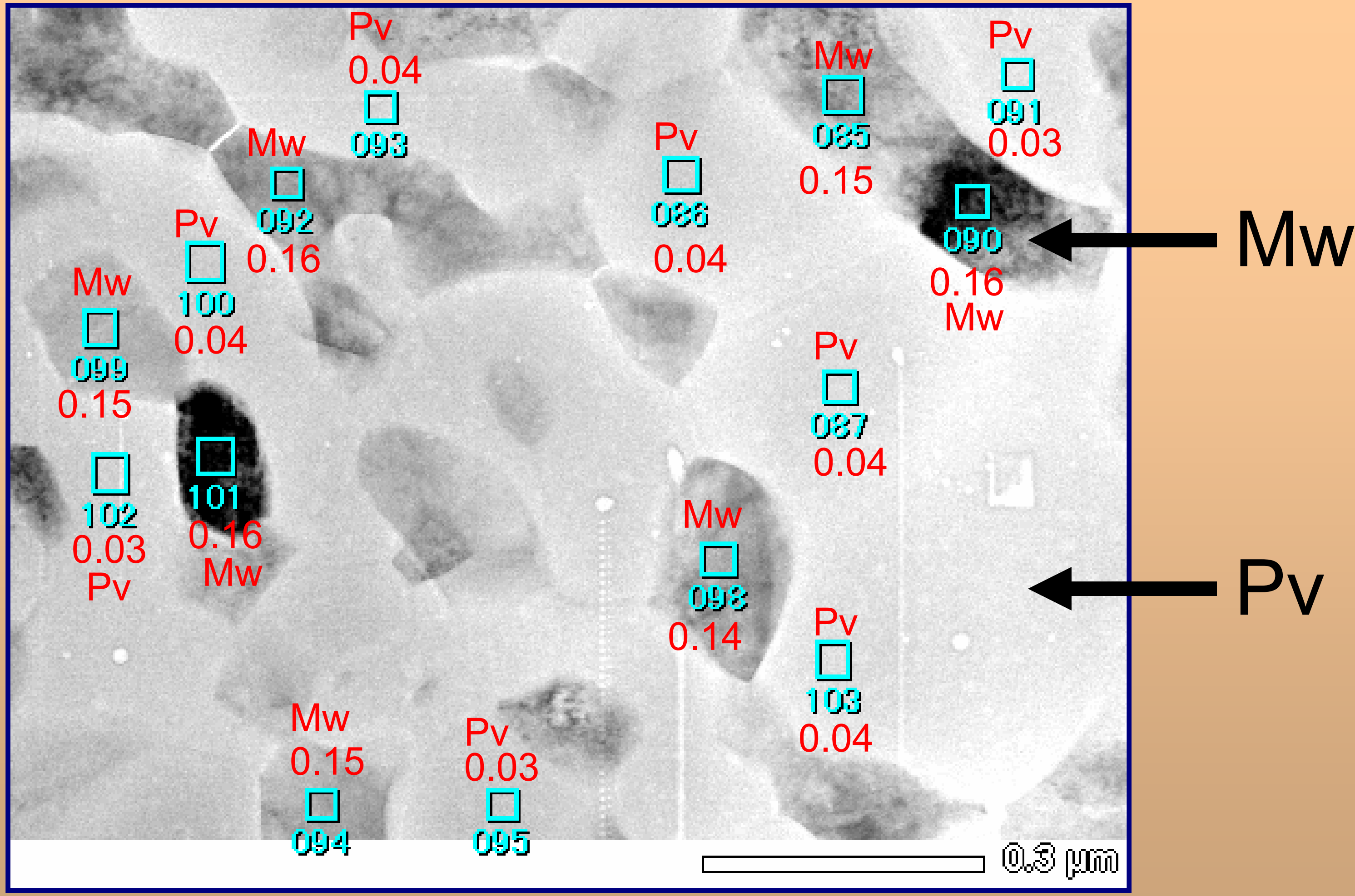
title

TEM image of the recovered sample



68GPa, 2000K
60min

High magnification image of the sample



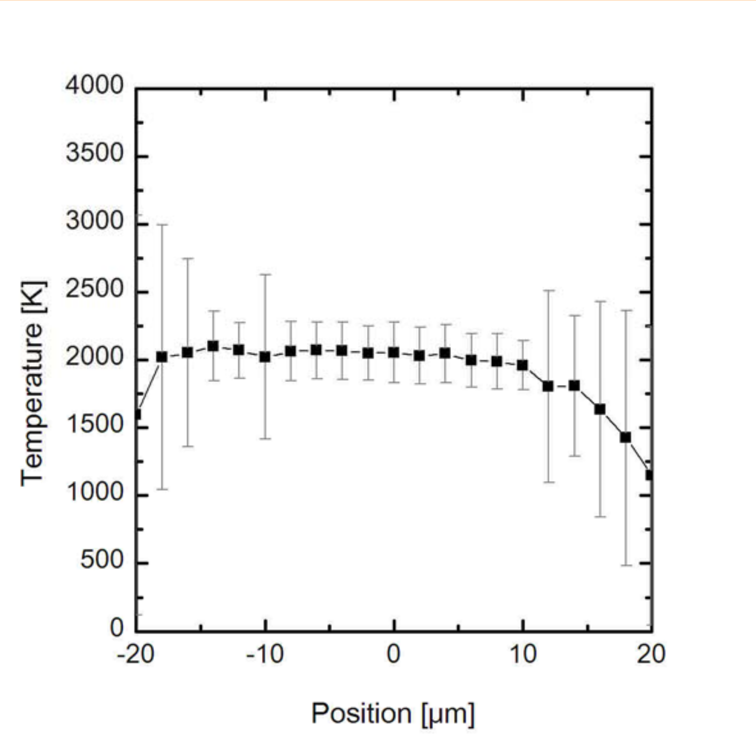


Fig. 2-3 Temperature distribution (Run SC34)

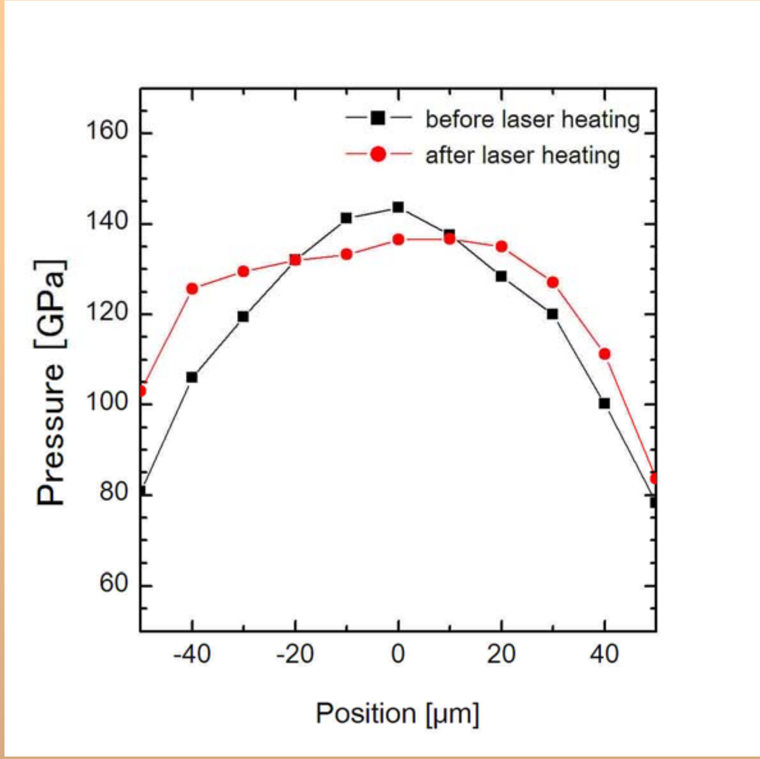


Fig. 2-2 Pressure distribution (Run SC34)

Table 2-1 The composition of San Carlos olivine

San Carlos Olivine							
n=5	wt.%	1σ	at.%	1σ	element	cation ratio	1σ
MgO	47.37	0.10	58.24	0.12	Mg	1.748	0.004
Al2O3	n.d.	-	n.d	-	Al	-	-
SiO2	40.37	0.10	33.29	0.08	Si	0.999	0.002
CaO	0.15	0.03	0.13	0.03	Ca	0.004	0.001
MnO	0.13	0.07	0.09	0.05	Mn	0.003	0.001
FeO	11.55	0.09	7.97	0.06	Fe	0.239	0.002
NiO	0.43	0.04	0.28	0.03	Ni	0.009	0.001
total	100.00		100.00		O	4	
Mg#			0.88		Cation sum.	3.001	0.005

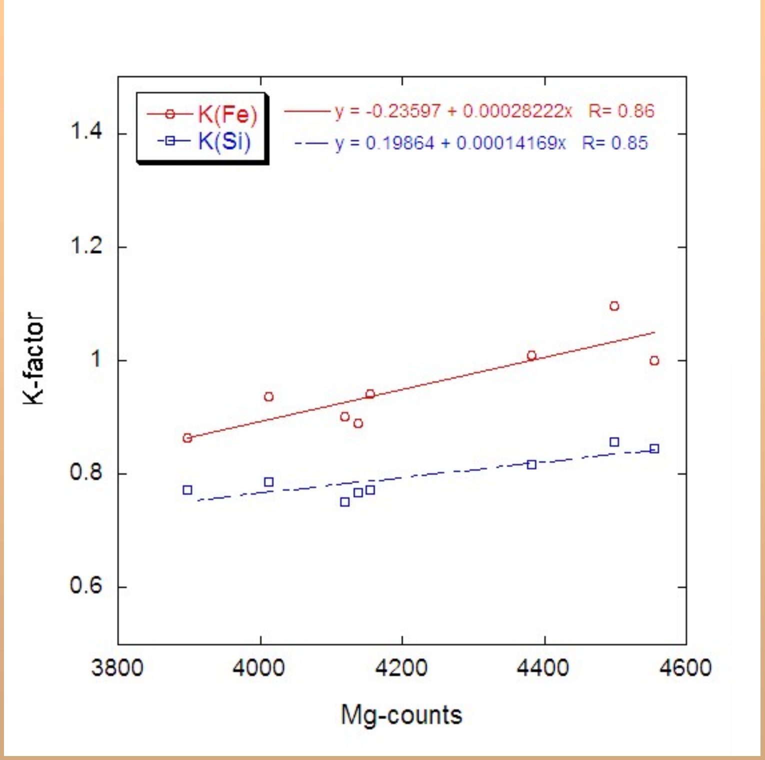
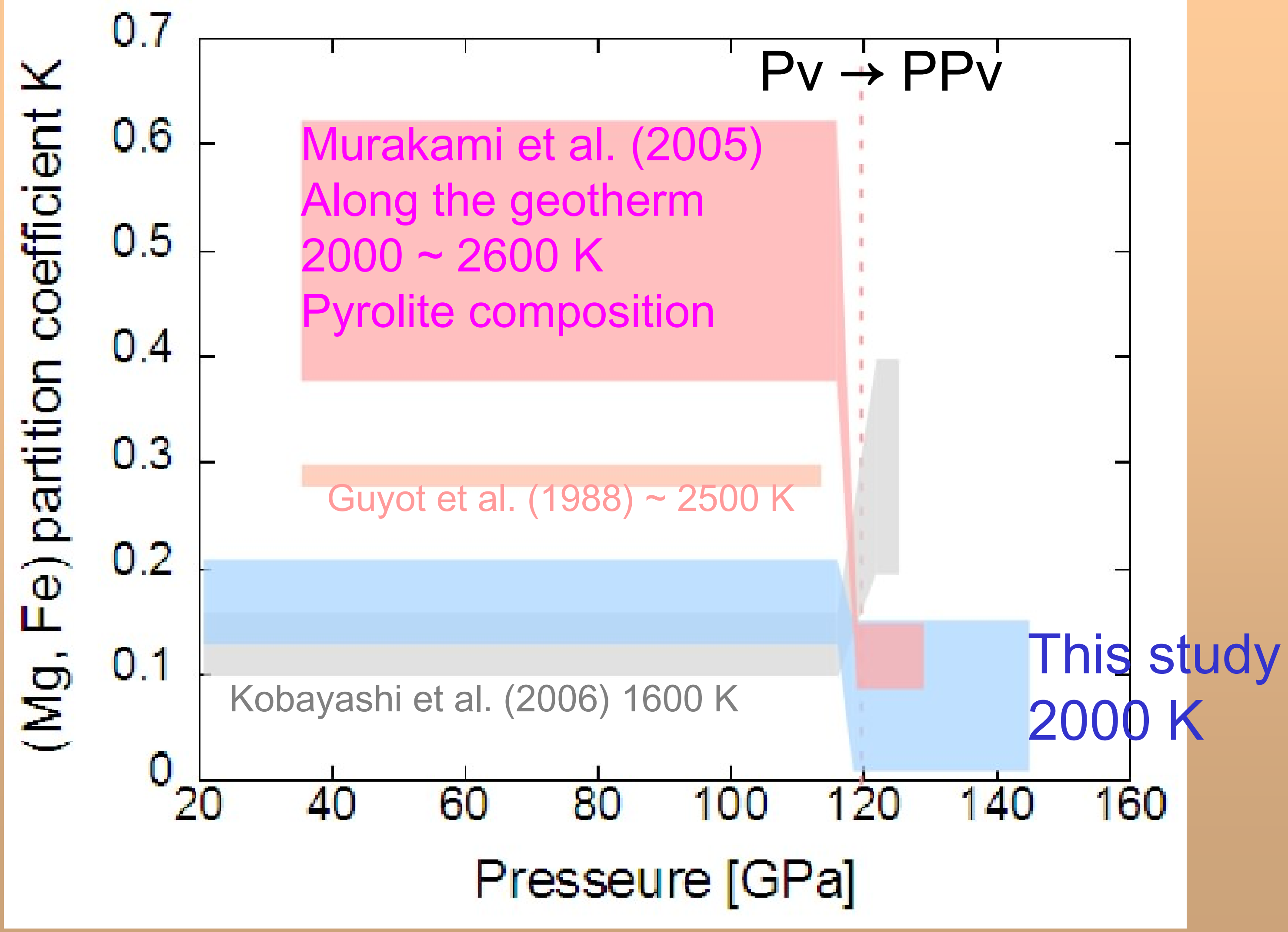


Fig. 3-4 The calibration curve of the k-factor of k_{FeMg} and k_{SiMg}

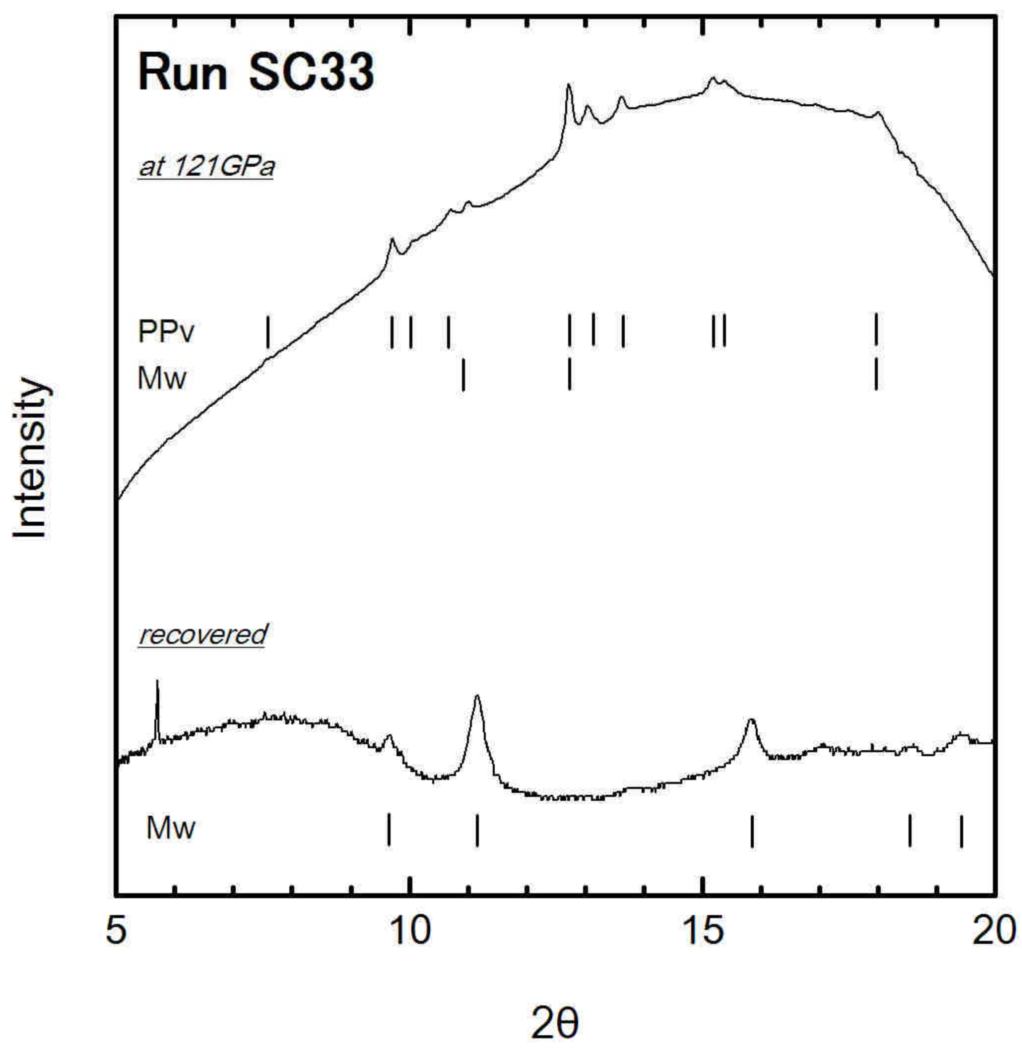
	Post-perovskite n=14		Ferropericlase n=12		Unheated area n=8	
wt.%						
MgO	44.34	2.55	55.12	1.38	47.70	0.52
Al_2O_3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
SiO_2	54.50	4.25	(sub)	(sub)	40.66	0.63
FeO	1.16	0.69	44.88	2.46	11.64	0.36
total	100.00	5.00	100.00	2.82	100.00	0.89
at.%						
MgO	54.37	3.12	68.64	1.72	58.52	0.64
Al_2O_3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
SiO_2	44.83	3.50	(sub)	(sub)	33.47	0.52
FeO	0.80	0.47	31.36	1.72	8.01	0.25
total	100.00	4.71	100.00	2.43	100.00	0.00
Fe#	0.01	0.01	0.31	0.02	0.12	0.01

Table 3-3 The composition of post-perovskite and ferropericlase (Run SC34)



Pv → PPv
Murakami et al. (2005)
Along the geotherm
2000 ~ 2600 K
Pyrolite composition
Guyot et al. (1988) ~ 2500 K
Kobayashi et al. (2006) 1600 K
This study
2000 K
(Mg, Fe) partition coefficient K
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
20
40
60
80
100
120
140
160
Presseure [GPa]

Powder X-ray diffraction pattern



121(2)GPa
2000(200)K
60min
After laser heating

recovered

Run		P [GPa]	Pv or PPv Fe#	err	Mw Fe#	err	Bulk Fe#	err	K	err
SC44	X- ray	**43**	**0.03**	0.01	**0.12**	0.02	**0.07**	0.02	**0.19**	0.07
SC40	X- ray	**73**	**0.04**	0.00	**0.16**	0.03	**0.10**	0.03	**0.21**	0.05
SC45	X- ray	**99**	**0.08**	0.01	**0.22**	0.01	**0.15**	0.01	**0.32**	0.05
SC33	X- ray	**121**	**0.03**		**0.21**	0.02	**0.12**	0.02	**0.14**	0.01
SC34	ATEM	**140**	**0.01**	0.01	**0.31**	0.03	**0.16**	0.03	**0.02**	0.02
SC41	X- ray	**154**	**0.01**		**0.23**	0.01	**0.12**	0.02	**0.02**	0.00