Trace elements in silicate melts at high pressure

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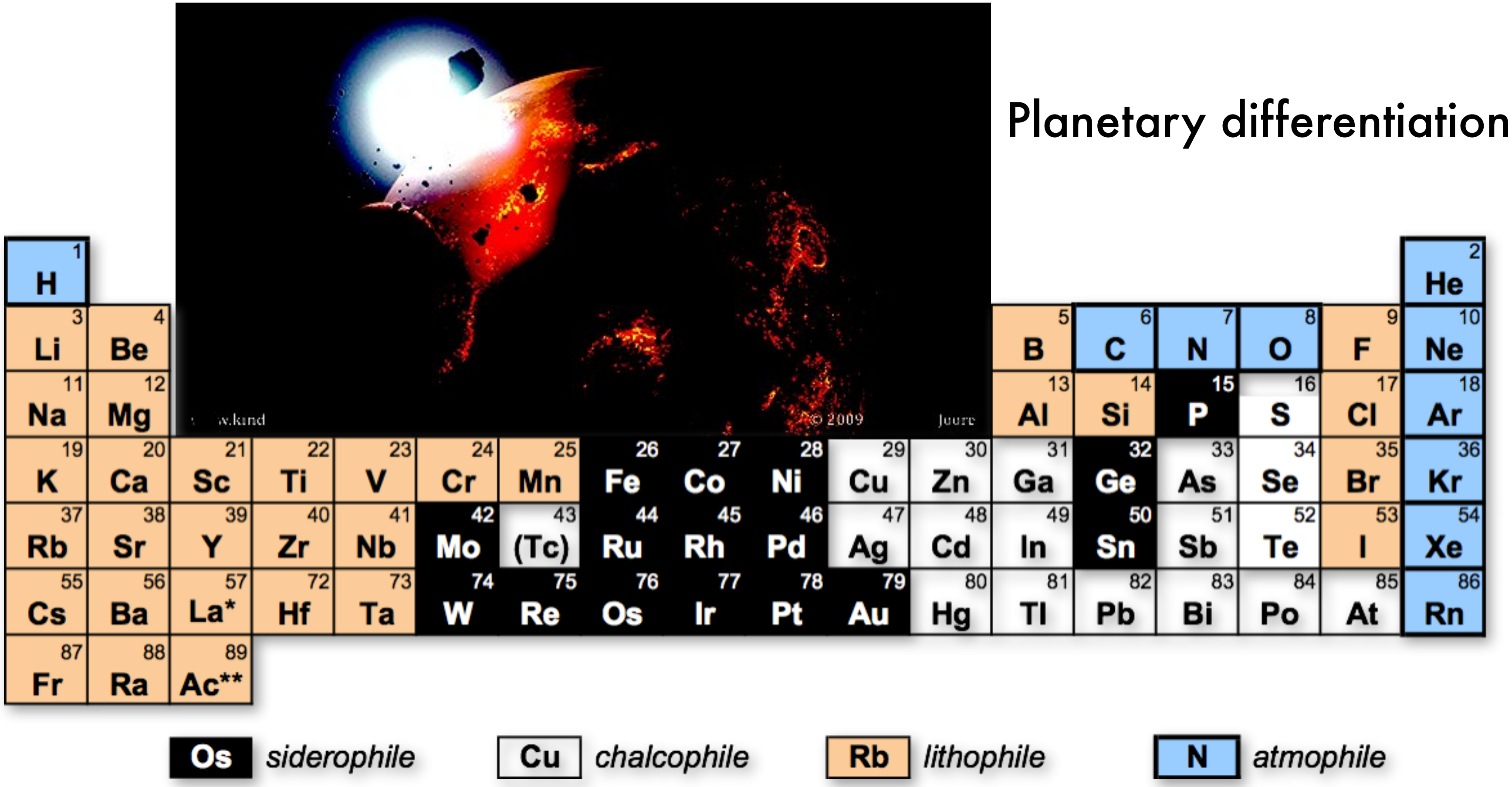
ELEMENT DISTRIBUTION DURING PLANETARY MELTING



Planetary differentiation

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 (Tc)	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac**															

Os *siderophile* **Cu** *chalcophile* **Rb** *lithophile* **N** *atmophile*

Does pressure affect the geochemical affinity of elements with silicate melts?

→ compatible/incompatible: crust formation ^{176}Lu/^{176}Hf, ^{146}Sm/^{142}Nd, ^{182}Hf/^{182}W

→ lithophile/volatile: atmosphere formation ^{129}I/^{129}Xe

Exploring silicate melt structure at high P-T conditions

Informations:

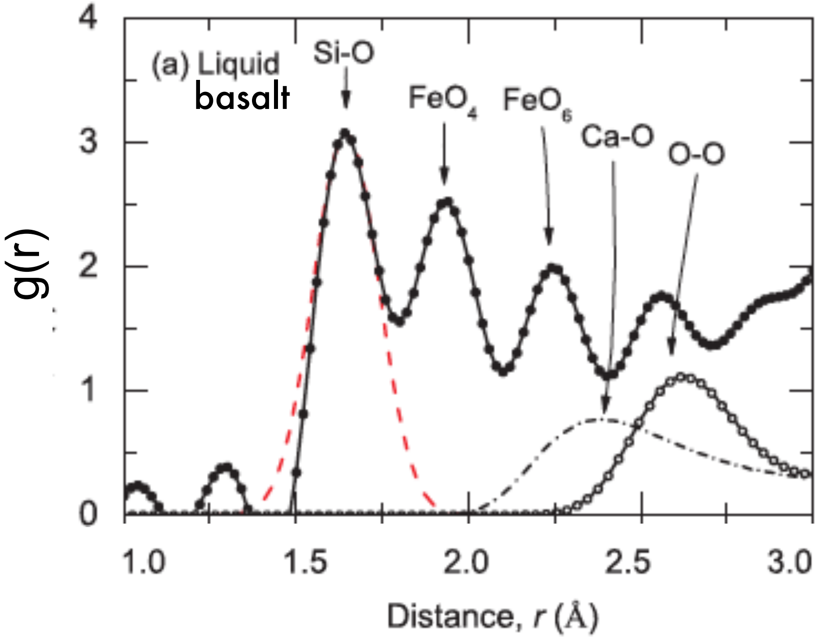
1) First coordination shell: interatomic distance, nature of neighbouring atoms, coordination number, oxidation state

2) mid-range order (XRD), second coordination shell (XRD, XAS)

X-ray diffraction:
All elements contribute to signal

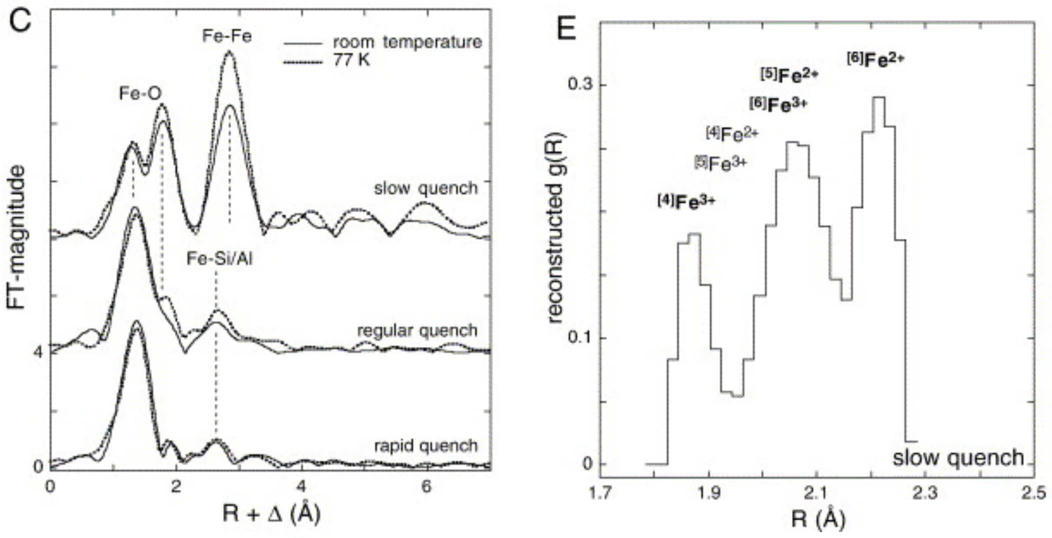
X-ray absorption spectroscopy:
Chemically selective, model dependent

Drewitt et al., PRB 2013.



Wilke et al., Chem. Geol. 2006.

Alumino-silicate glass



Trace and minor elements in magmas: experimental approaches

X-ray diffraction:
All elements contribute to signal
Restrictions: only very heavy elements
Fe-free compositions

Elements: Lu, Nd, Xe

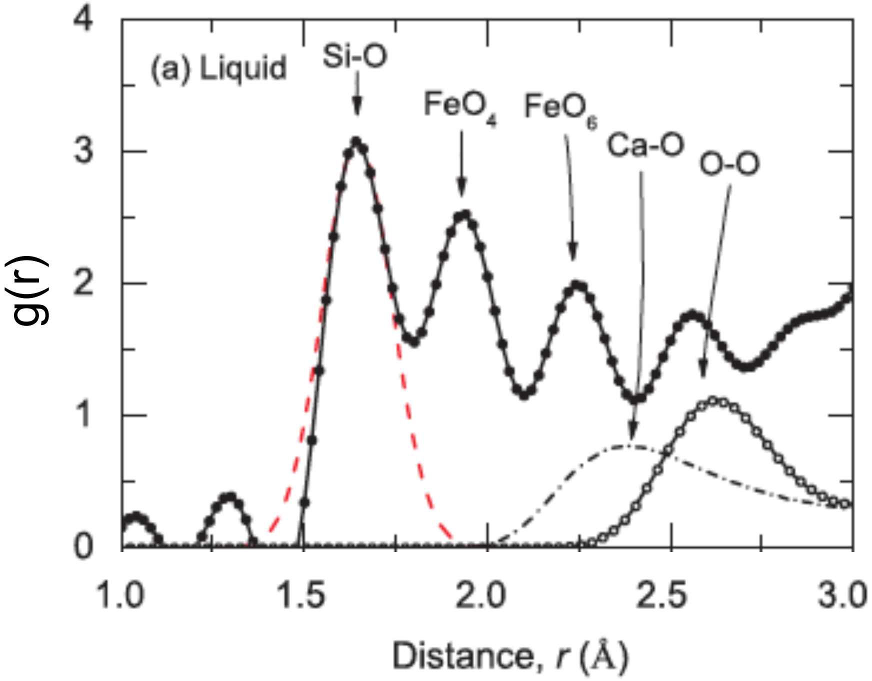
X-ray absorption spectroscopy:
Chemically selective, model dependent
Restrictions: 11 keV < energy < 30 keV

Elements: W, Nb, Br, Kr

Major oxide components in silicate melts:

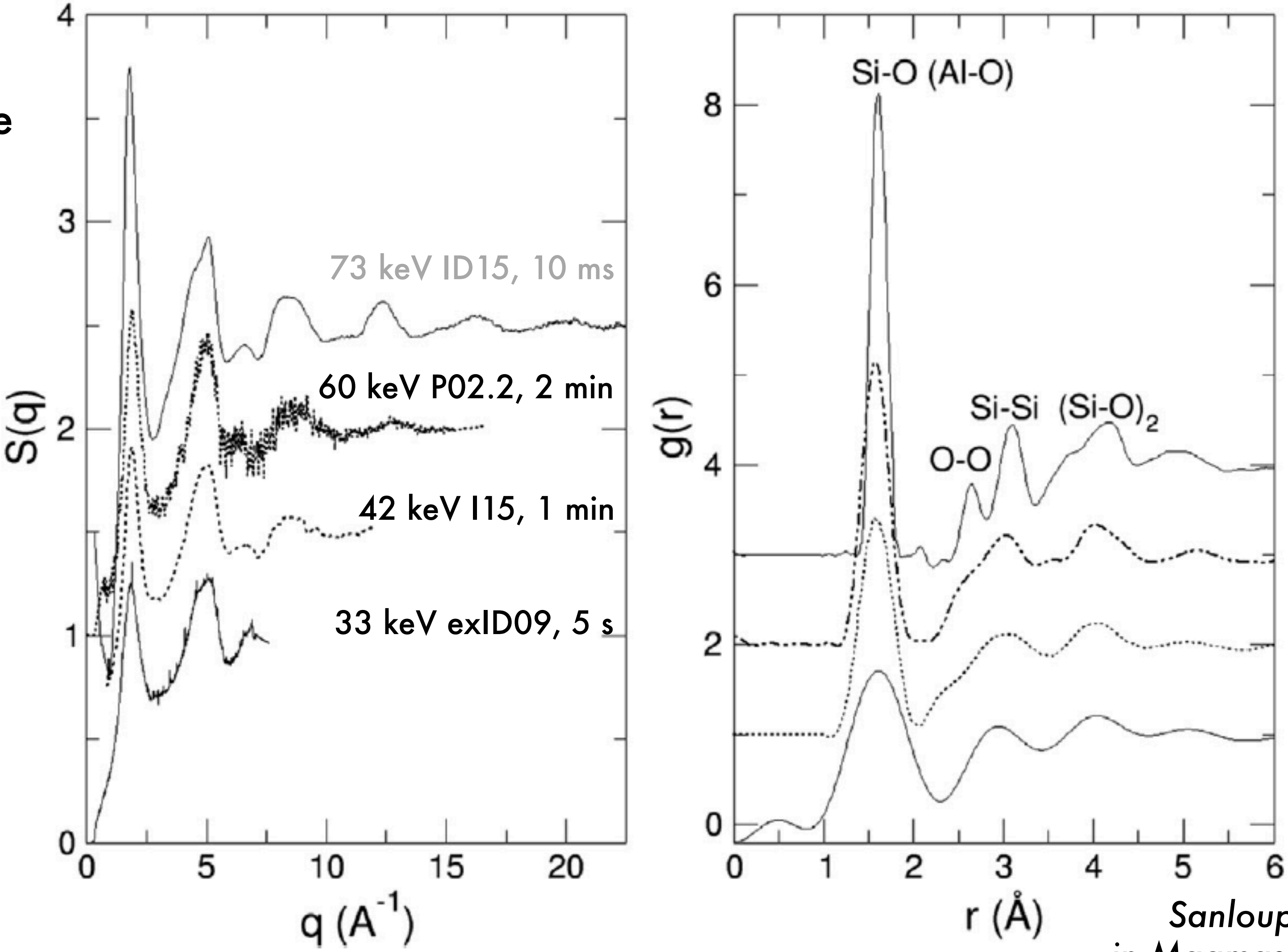
	SiO_2	Al_2O_3	FeO	MgO	CaO	Na_2O	K_2O	H_2O
granite	76%	13%	2%	0.5%	2.5%	3%	2%	
haplogranite	68%	11%	-	-	-	4%	3%	15%
basalt	50%	15%	8%	8%	13%	2%	2%	

Drewitt *et al.*, *PRB 2013*.



Probing trace elements in melts at high P-T conditions using XRD

Molten
haplogranite
in RH-DAC
Or ambient
P-T glass



73 keV ID15, 10 ms

60 keV P02.2, 2 min

42 keV I15, 1 min

33 keV exID09, 5 s

Ideal but
impossible now
at high P

Best at high P

Possible at high P

Insufficient
resolution

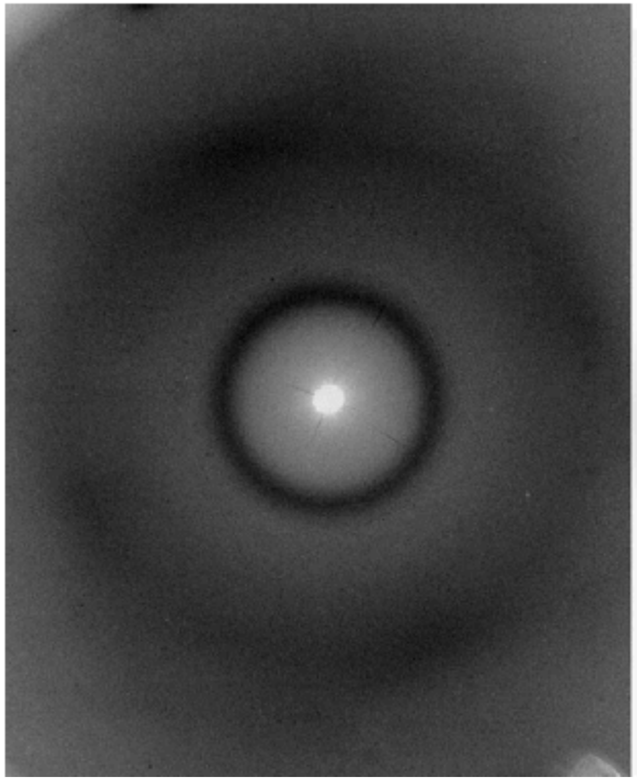
Sanloup and de Grouchy,
in Magmas under pressure 2018.

Window between 1.8-2.5 Å: where many key trace elements are expected

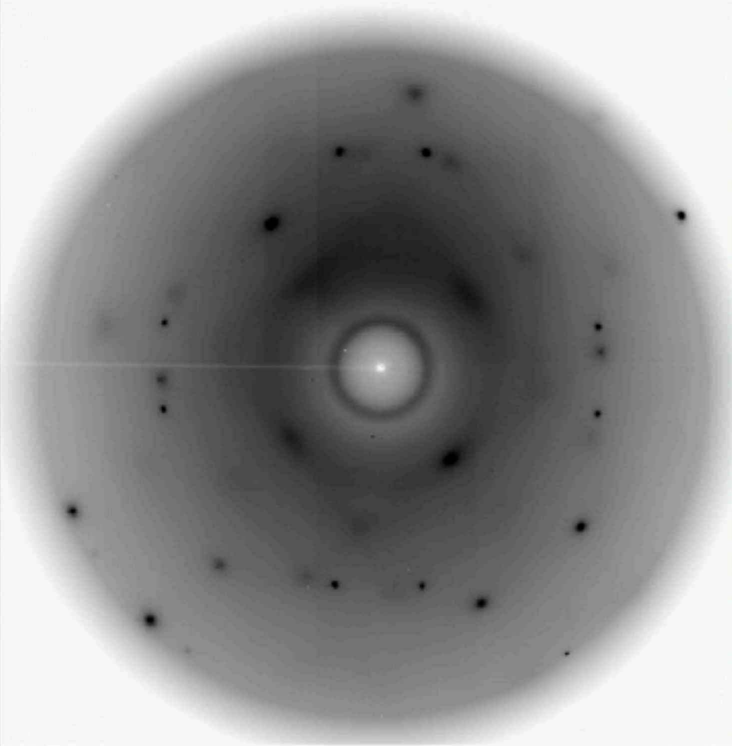
Requirement of a sufficiently large q-range:
high-energy angle dispersive XRD in DACs or energy dispersive XRD in large volume presses

Probing trace elements in melts at high P-T conditions using XRD

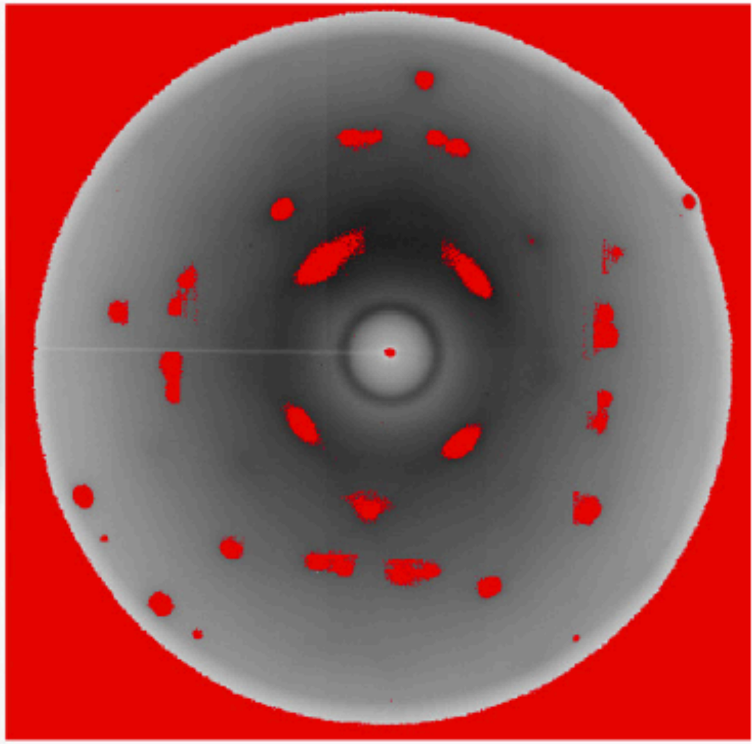
Angle-dispersive x-ray diffraction and DACs:
correction for diamonds Bragg peaks is significant at high energies



33 keV, MAR555



60 keV, Perkin-Elmer

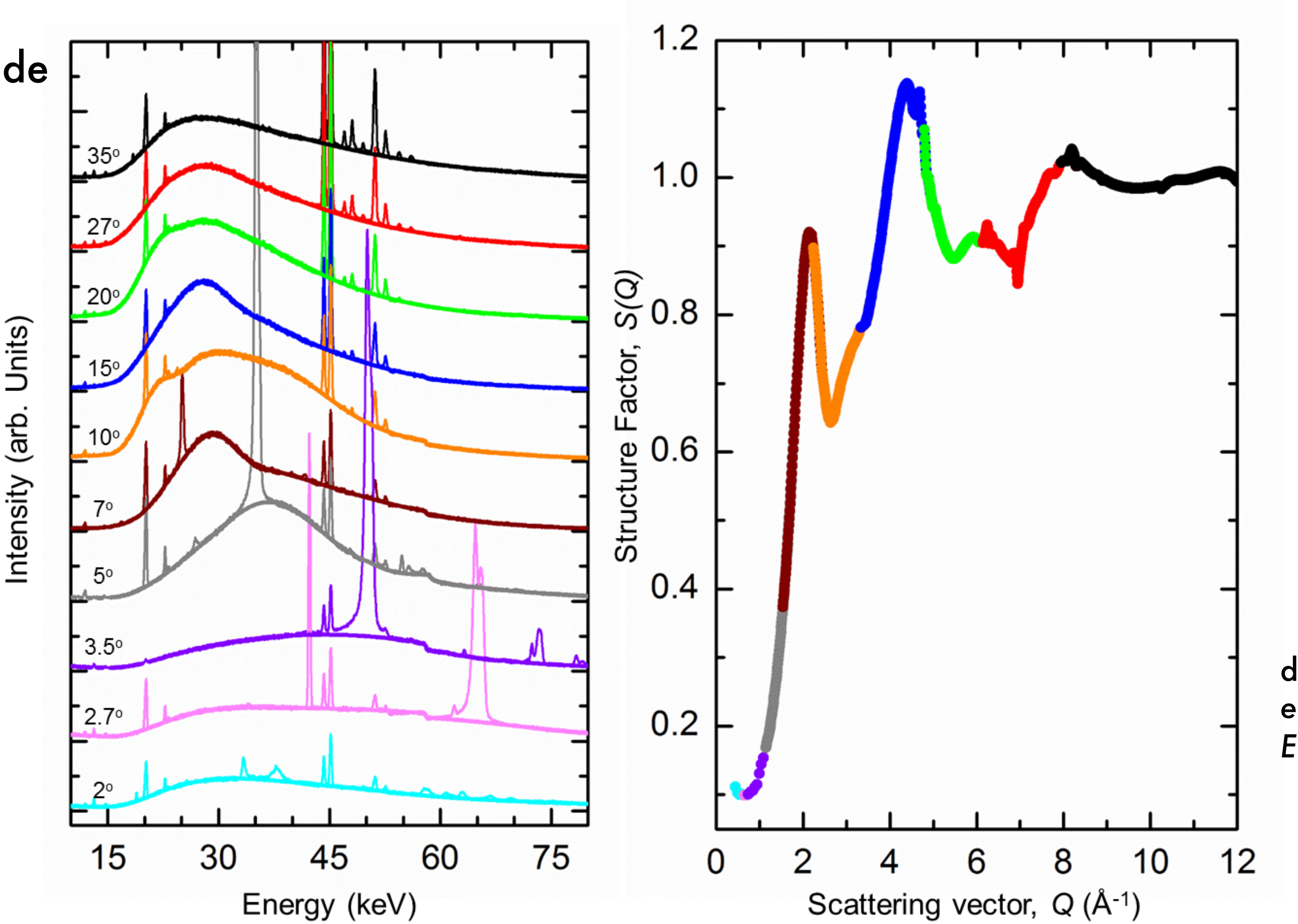


Probing trace elements in melts at high P-T conditions using XRD

Energy-dispersive x-ray diffraction and large-volume press

Anorthite-diopside melt + Lutetium

APS, HPCAT, 16BM-B



de Grouchy *et al*, *EPSL 2017*

NB: some elements may have strong fluorescence peaks that need to be removed

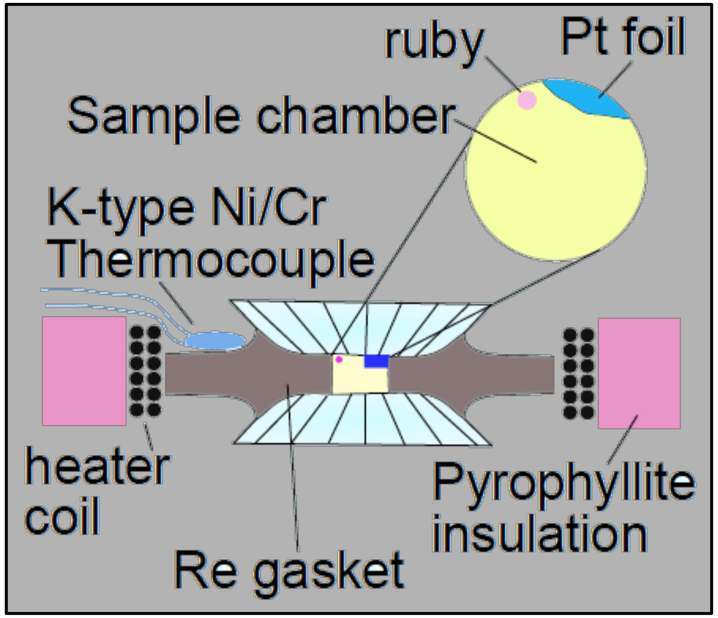
Exploring silicate melt structure at high P-T conditions

Resistive heating DACs:

Optimizing sample volume

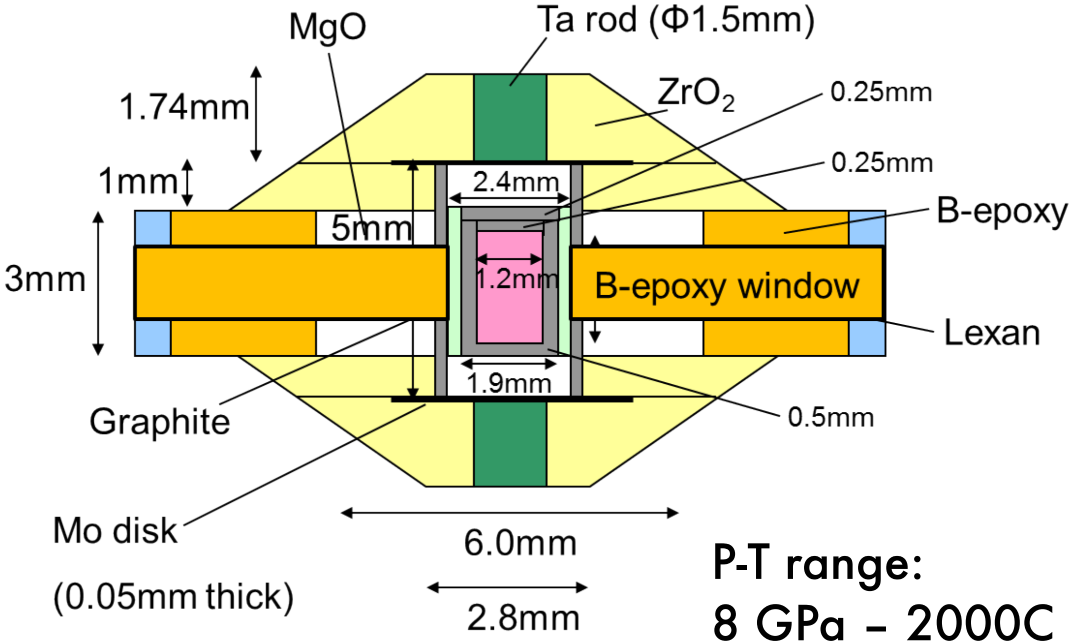
Large opening DACs, *e.g.* Boelher-Almax anvils

Need hydrated glasses to lower melting T



Paris-Edinburgh press:

Same cell-assembly used for XRD and XAS (provided by the APS)



P-T range:
8 GPa – 2000C

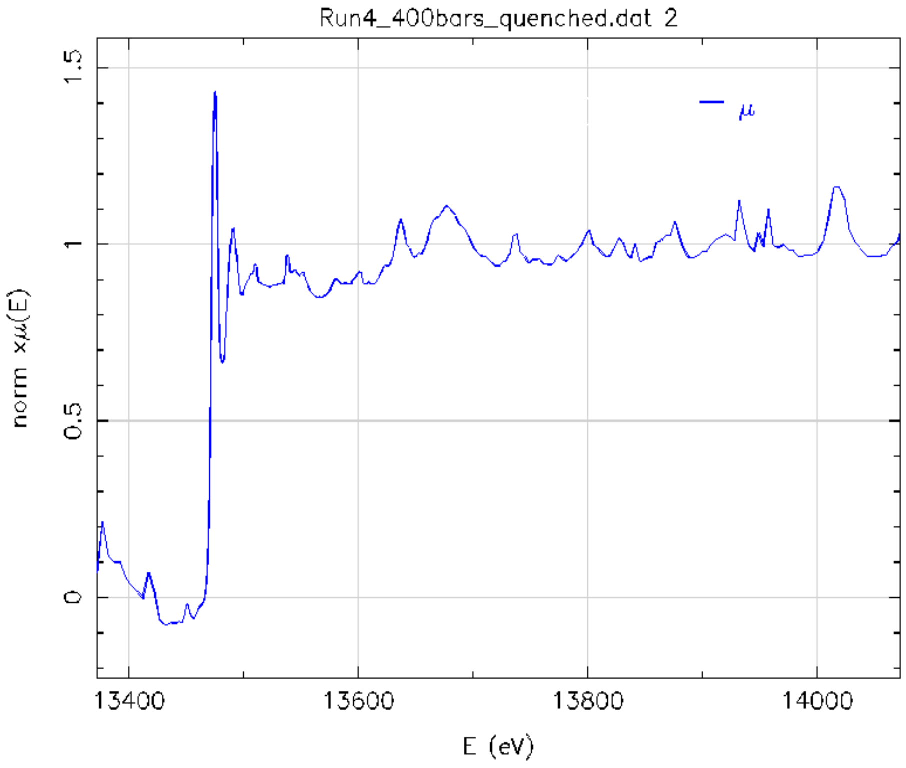
High stability at high T, large vertical access

X-ray absorption spectroscopy at high P-T conditions

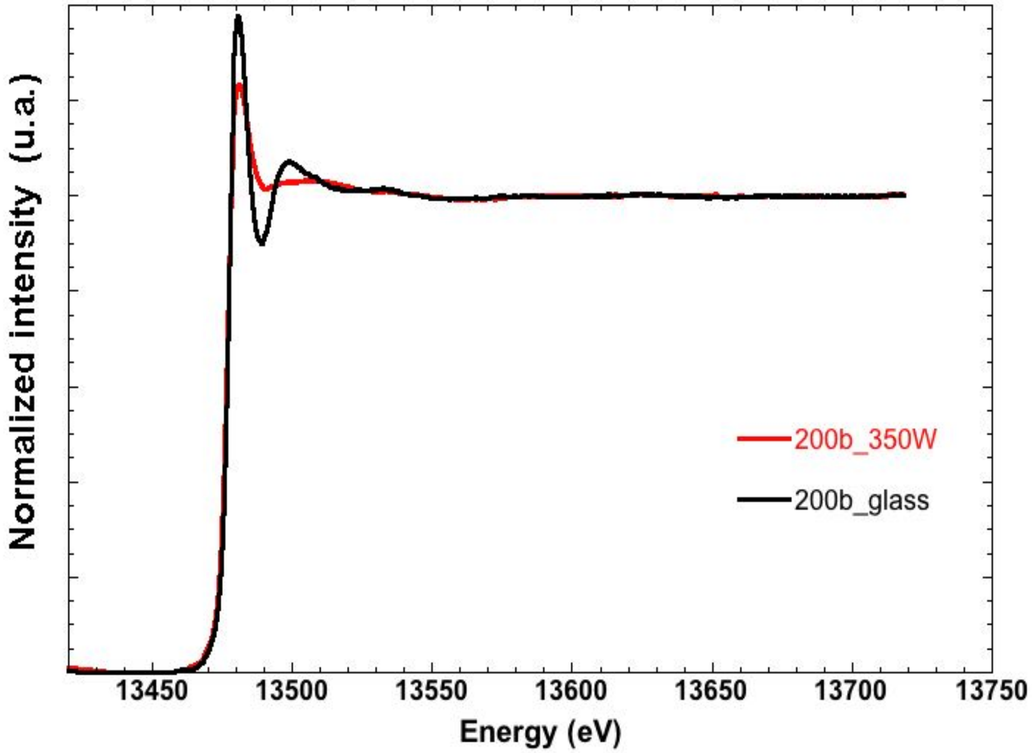
Requires nanocristalline diamond capsules or anvils
PRIUS programme, GRC Ehime University (Pr. Irifune)

Br-dopped (0.4 at%) dacitic melt

Using polycrystalline diamond capsules
(Almax)



Using nanocristalline diamond capsules
(Ehime)

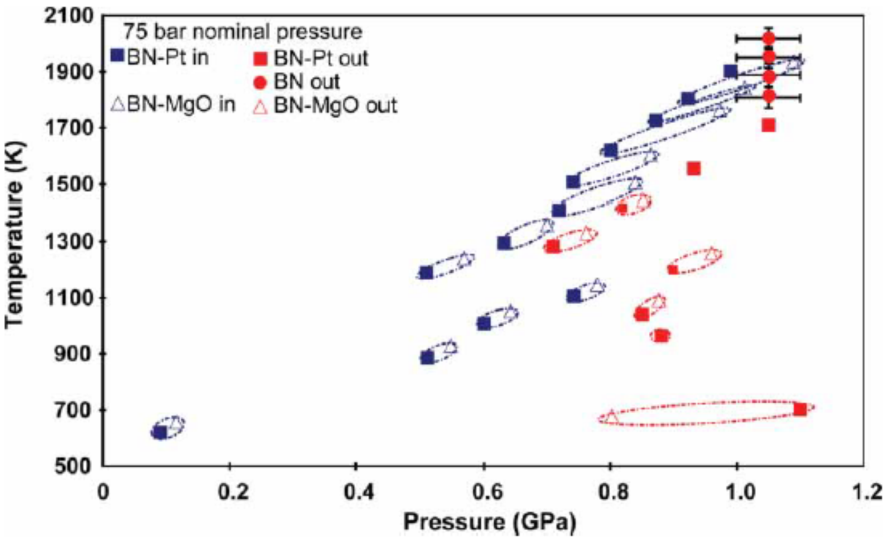


Cochain et al. *Chem Geol* 2015

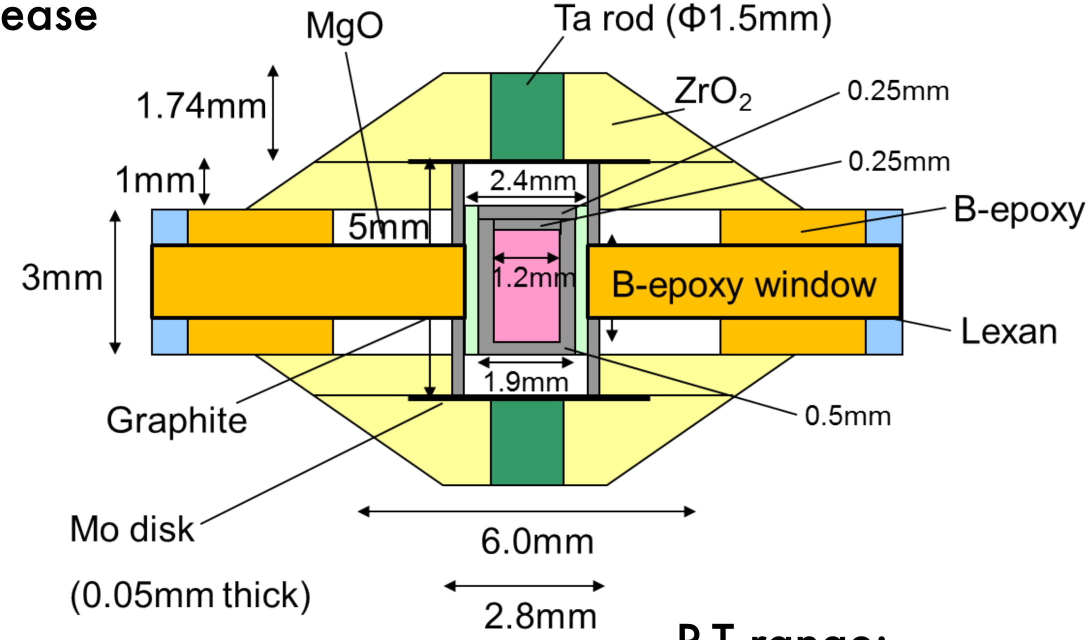
X-ray absorption spectroscopy using a Paris-Edinburgh press

Long collection times (3 hours) ⇒ Need high stability cell-assembly and large vertical gap to optimise signal/noise ratio

Nanocristalline diamond capsules
⇒ Need to raise T above 1000 ℃ for P increase



van Kan Parker et al., High Press. Res. 2010.

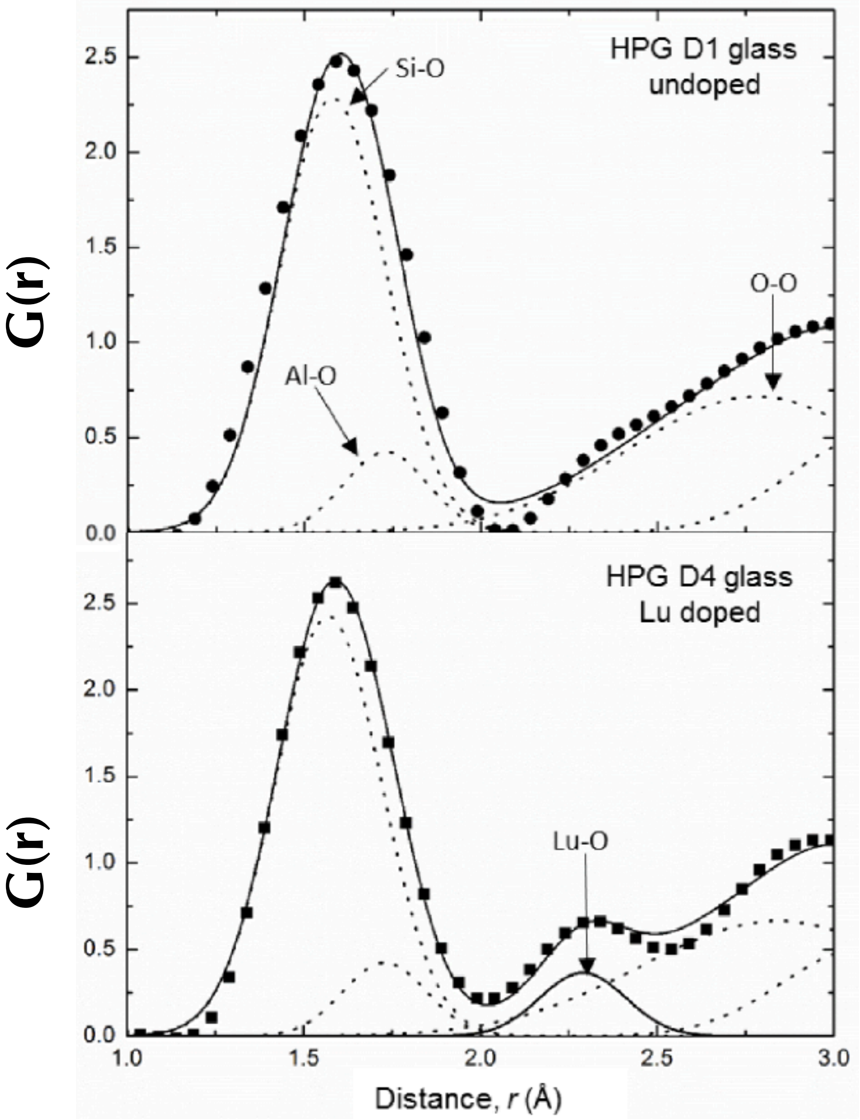


P-T range:
8 GPa – 2000 ℃

Use of Pt-Rh or graphite caps:
Possibility to buffer the redox state (also talc powder outside caps)

Lutetium - X-ray diffraction in DACs (Diamond, I15) and PE press (HPCAT)

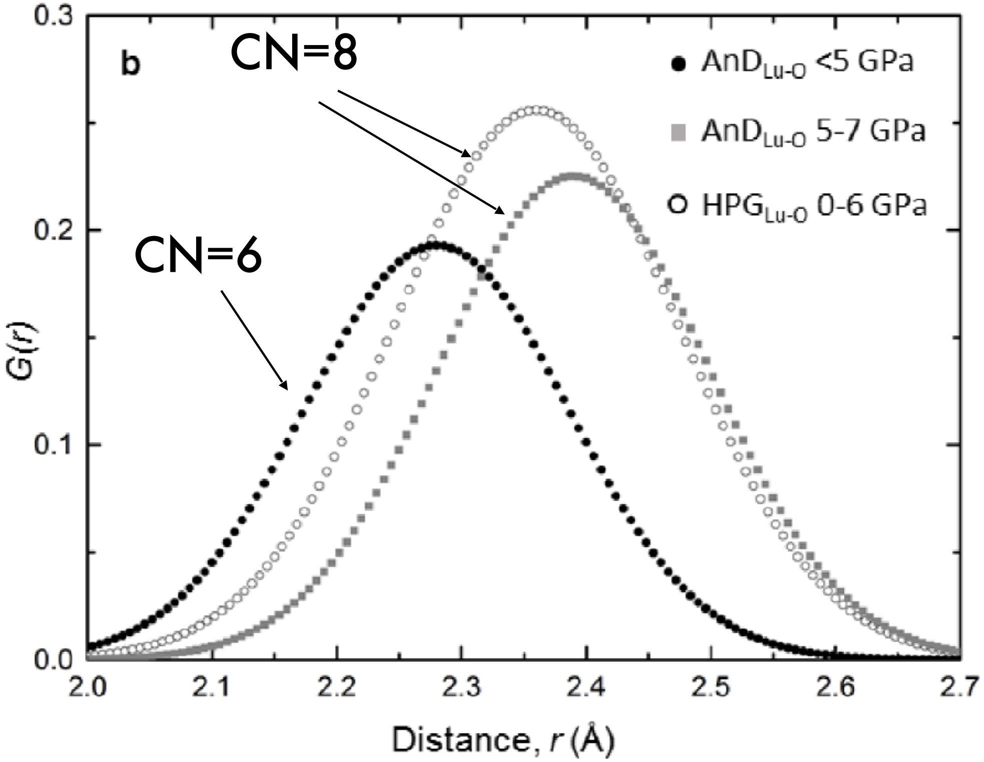
de Grouchy *et al, EPSL 2017*



An-D: Fe-free basalt analogue

HPG: Fe-free granite analogue

Fit of the Lu-O contribution:

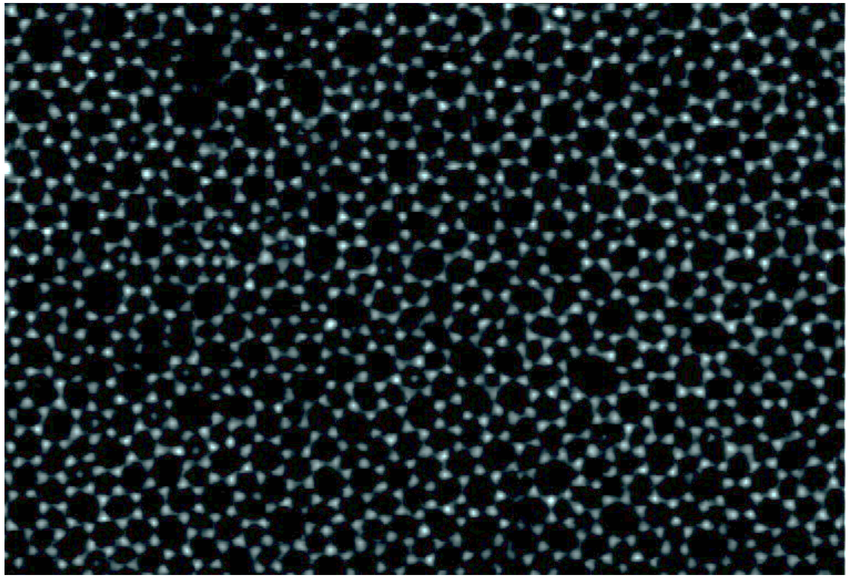


⇒ **Lu-O coordination change in basalts: from 6 to 8 at 4-5 GPa**

Changes of environment of Lu, Nd in melts at high P: summary

- Lu-O: CN changes from 6 to 8 at ~4-5 GPa
- Coincides with change of P-dependence in crystal/melt partitioning

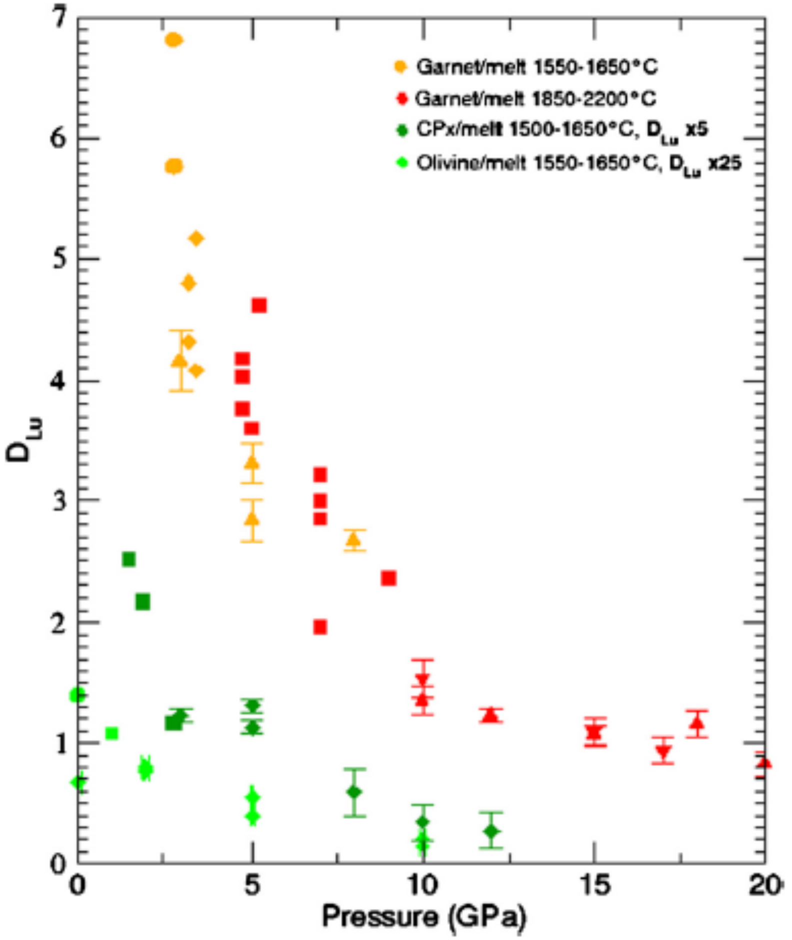
- Nd-O: CN changes from 6 to 8 at ~1-2 GPa



SiO$_2$ glass layer, TEM

Huang et al., *Nano Lett.*, 2012

de Grouchy et al., *EPSL* 2017



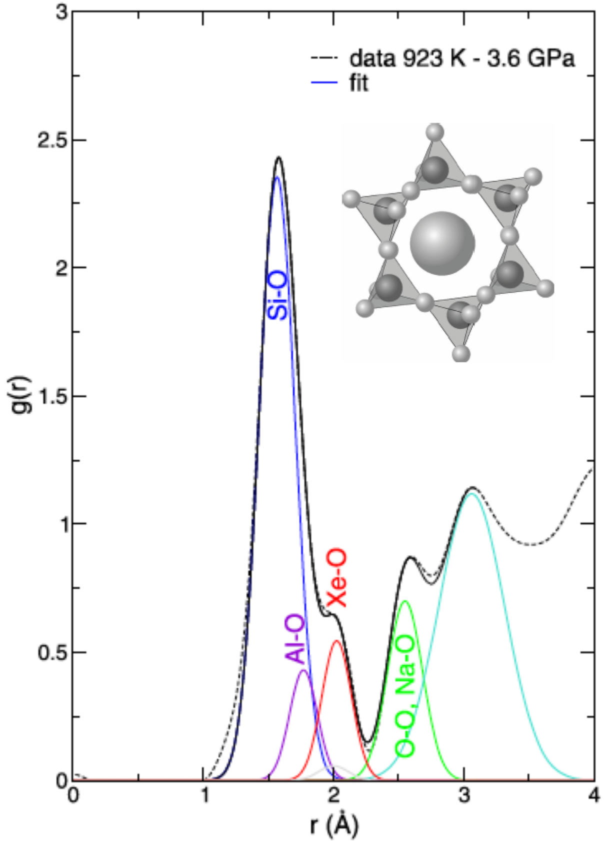
⇒ D_{Lu}/D_{Hf} ~ 1 above 5 GPa: Lu and Hf should not be fractionated in high P basalts

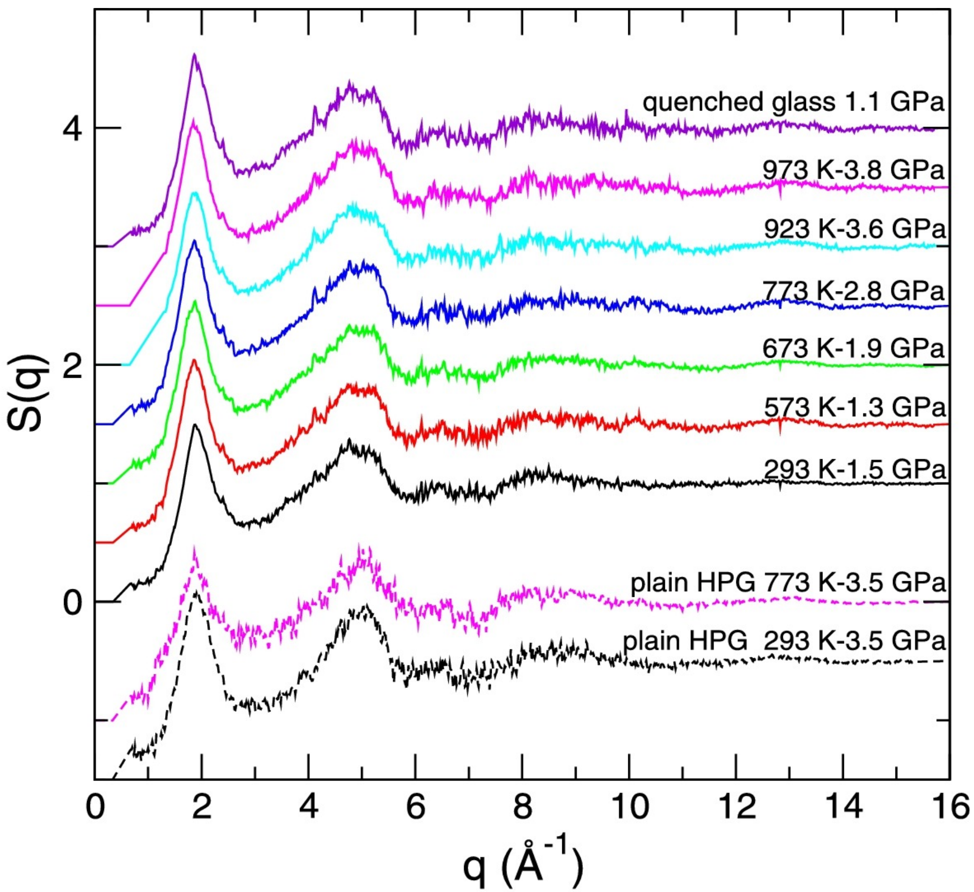
⇒ Decoupling of Lu/Hf and Nd/Sm systems for high P melts

Reactivity of xenon and krypton in magmas

X-ray diffraction @ 60 keV, PetraIII (Hambourg)

Haplogranite melt





Xe-O = 2.1±0.1 Å

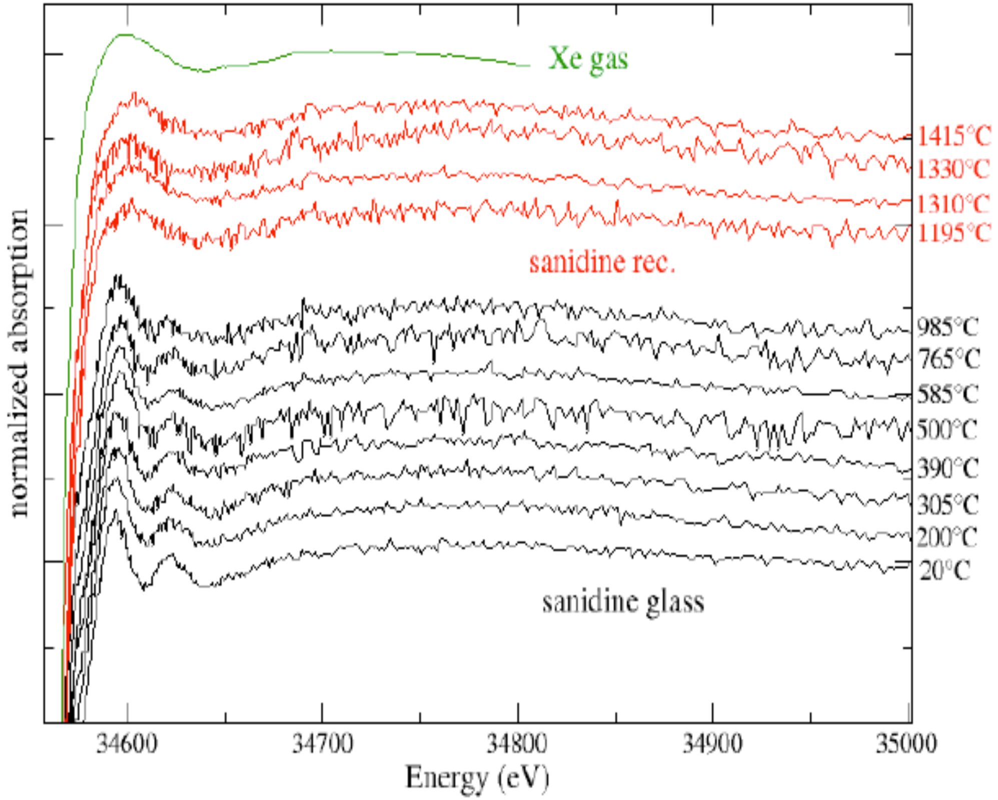
⇒ similar distance in crystals, but different CN

Leroy et al. *EPSL* 2018

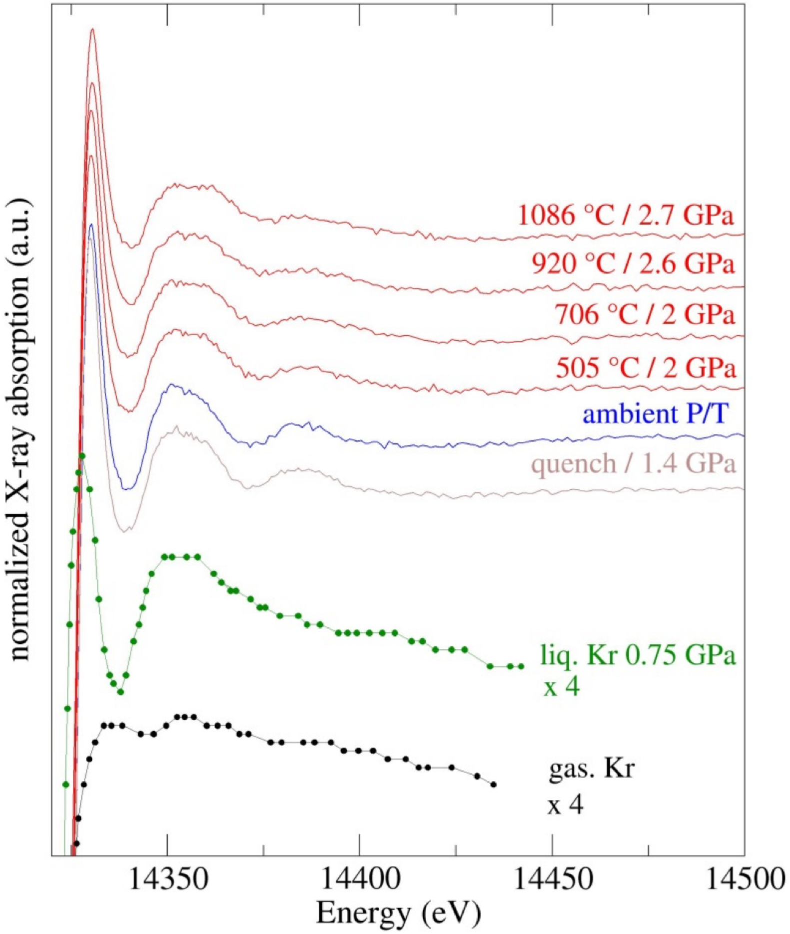
Reactivity of xenon and krypton in magmas

EXAFS, ESRF (BM23)
Glass and molten feldspar (sanidine) doped with Xe:Kr gas

Xe edge



Kr edge



Crépisson et al. *Chem Geol* 2018

Reactivity of xenon and krypton in magmas

EXAFS, ESRF (BM23)
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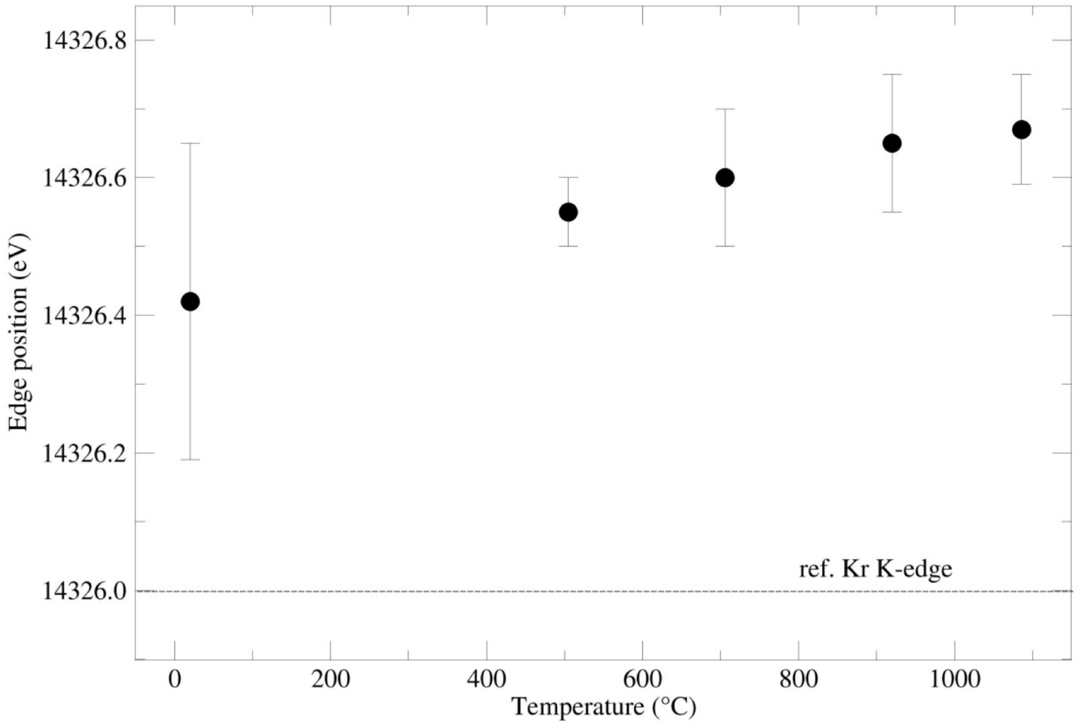
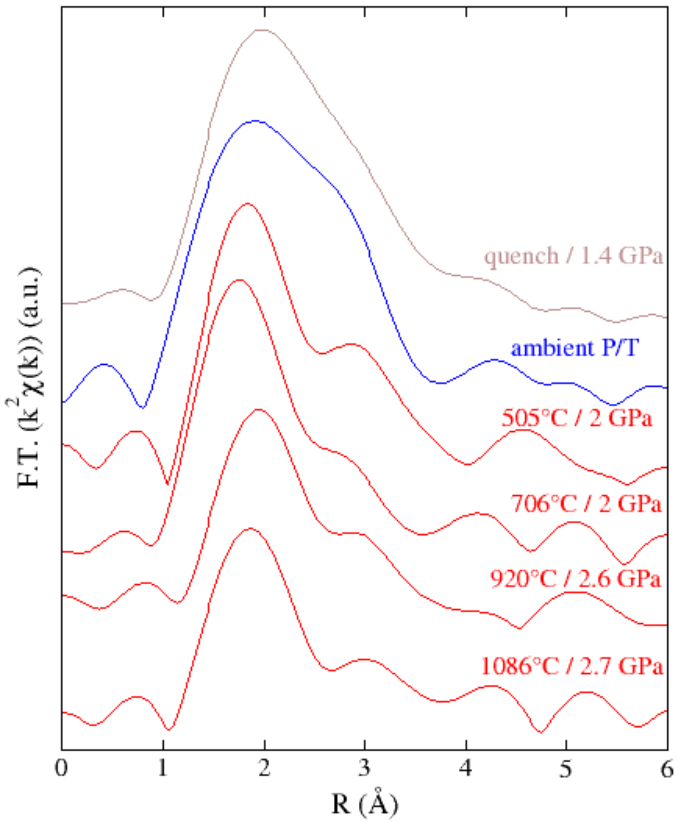




Kr-O = 2.5±0.1 Å

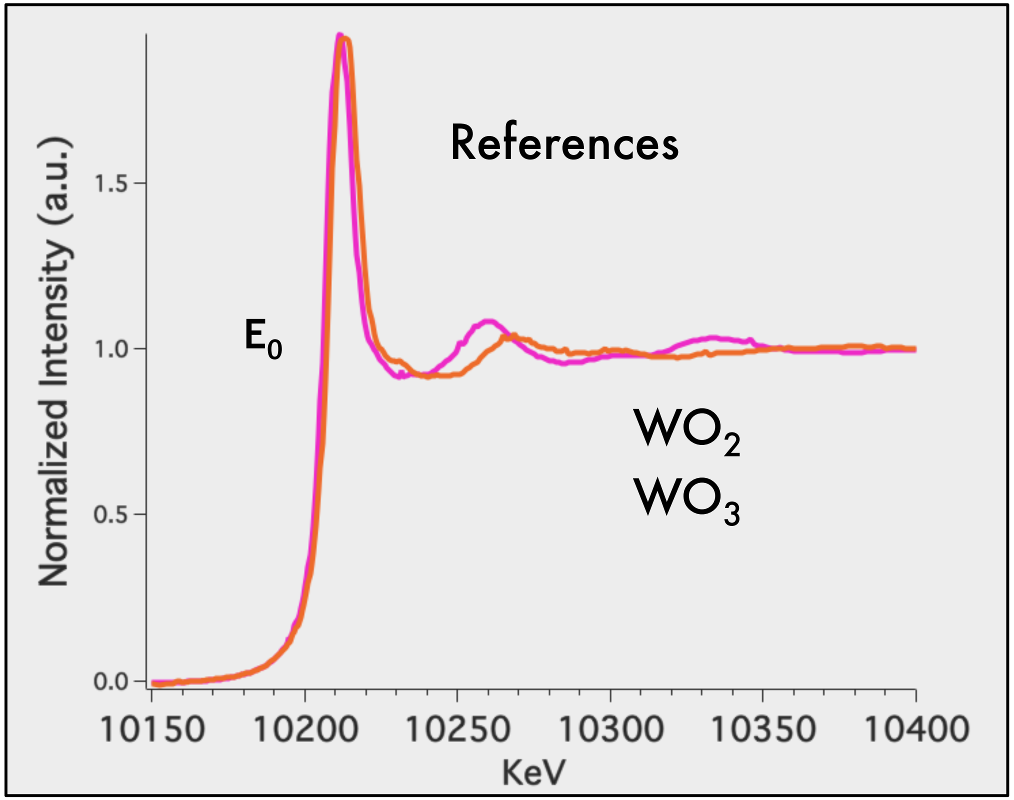
⇒ Kr also gets oxidized under pressure

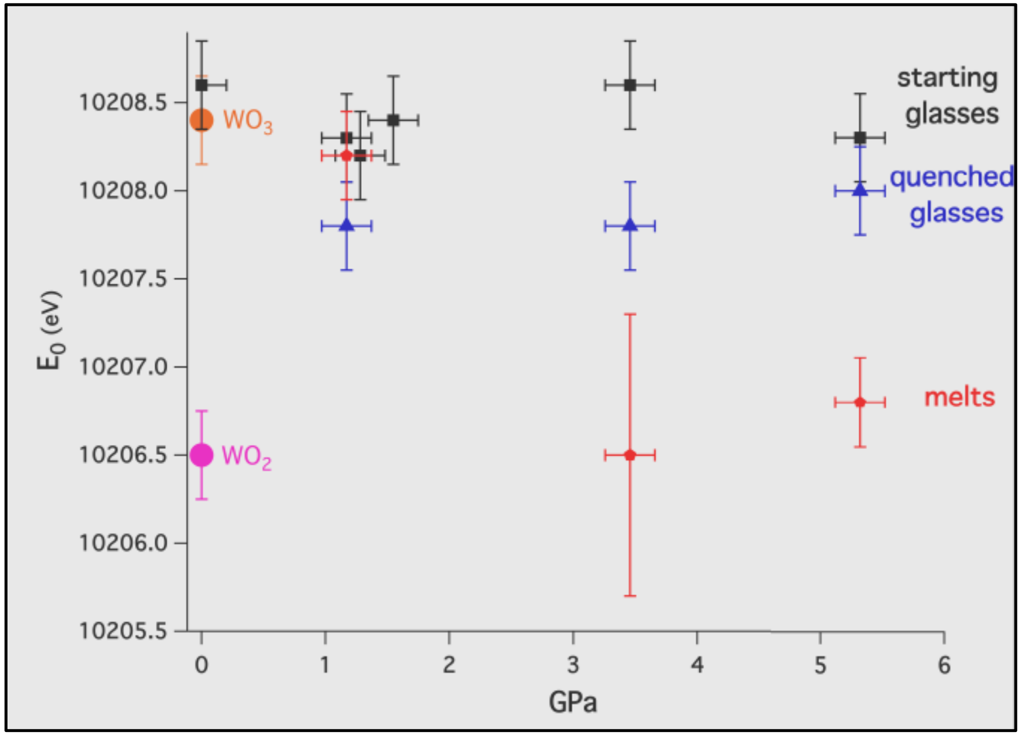
Crépisson et al. *Chem Geol* 2018

Tungsten - X-ray absorption in Paris-Edinburgh press (ESRF, BM23)

Basalt +0.6 wt% W

- Current debate on change from W^{6+} to W^{4+} with pressure



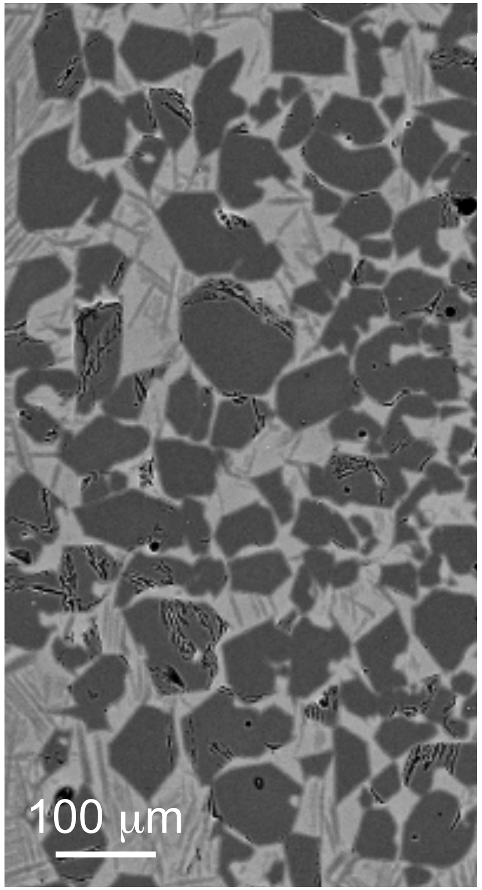


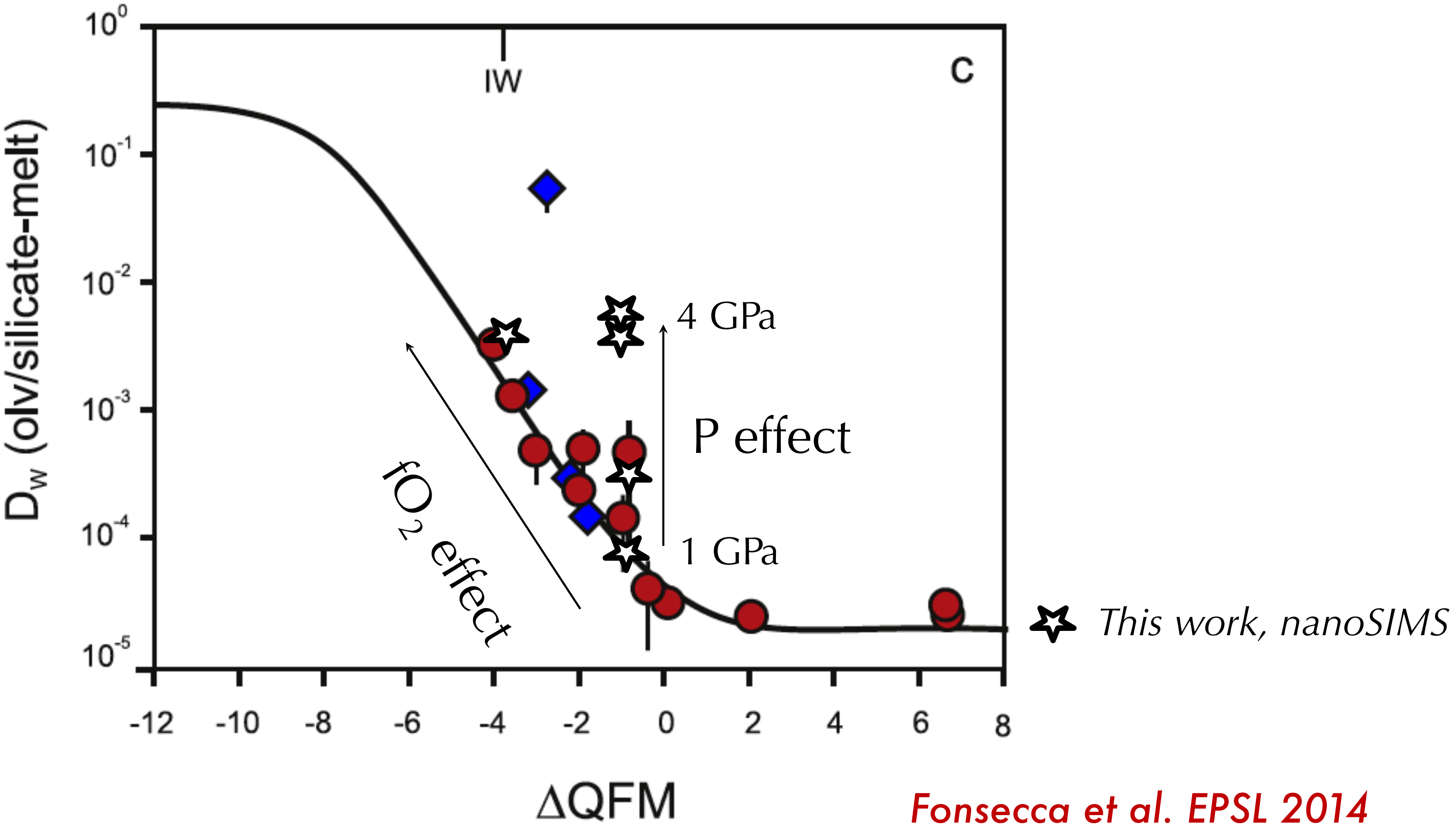
Cochain *et al. In prep.*

⇒ Reduction of W in the melt around 2-3 GPa

⇒ Not preserved in the quenched glass

Tungsten – Effect of oxidation state on partitioning





Fonsecca et al. EPSL 2014

Righter&Shearer, GCA 2003

⇒ High pressure residues have high [W]

Trace elements in melts: perspectives opened by the EBS

X-ray diffraction:
Currently limited to upper mantle studies for trace elements

EBS:
Much shorter collection times at high energy (>60 keV)
Better focussing at high energy
⇒ compatible with laser heating DAC

X-ray absorption spectroscopy:
Chemically selective, model dependent
Restrictions: 11 keV < energy <30 keV

EBS:
Higher energies accessible at high P-T
Real ‘trace’ elements studies instead of 1% concentrations, *i.e.* <0.1 at%

Eventually also using LH-DACs

⇒ Opens applications to the whole terrestrial P-T range

(i.e. deep mantle reservoirs, core formation) with natural concentrations

Thanks for provision of beamtime:
APS HPCAT 16BM-B, ESRF BM23, Diamond I15

Contributed to this work:

for synchrotron experiments:
D. Daisenberg[1], I. Kantor[2], Y. Kono[3], Z. Konopkova[4], K. Glazyrin[4], A. Rosa[2]

for nano-SIMS analysis:
M. Roskosz[5]

[1]Diamond Light Source, [2] ESRF,
[3] HPCAT, Carnegie Institution of Washington now at Ehime University,
[4]DESY, [5]Museum National d'Histoire Naturelle

Work funded by the
European Research Council
"Magmas at depth: an Experimental Study at
Extreme Conditions"