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Xenon compatibility in magmatic processes: Hadean to current contexts

Q. Chen¹, C. Sanloup^{1*}, D. Horlait², G. Shen³

Abstract





Xenon (Xe) behaviour in petrological processes, albeit essential to constrain mantle ingassing and degassing models, is elusive due to its volatile nature, and lack of direct investigation at the pressures (*P*) and temperatures (*T*) relevant to magma formation and crystallisation at depth. Xenon stands out amongst noble gases due to its unique reactivity with silicates of the lower crust and upper mantle, which could at least partially explain that published mineral/melt partitioning coefficients span up to six orders of magnitude. We report partition coefficients of Xe using *in situ* X-ray fluorescence at high *P* and *T*, and mass spectrometry analyses. Xenon is found to be moderately incompatible in anorthite-clinopyroxene mix in equilibrium with basalt (partition coefficient value of 0.16 ± 0.06), and compatible in olivine in equilibrium

with basalt (partition coefficients in the range 88 ± 22 to 302 ± 46). While Xe is, thus, concentrated in basaltic melts coexisting with crystallising pyroxenes and feldspars, it is strongly retained in olivine at depth. Consequently, Xe originally contained in solid Earth has been preferentially retained at depth throughout Earth's history, from the magma ocean stages to present day partial mantle melting processes.

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Introduction

Noble gases provide unique clues to unravel the geochemical evolution of volatile elements upon Earth's formation to present day geodynamics (Ozima et al., 2002 and references therein), assuming their inertness and volatile behaviour. Xenon is also unique for its enigmatic atmospheric depletion relative to lighter noble gases (Anders and Owen, 1977), known as the 'Xe paradox', and its strong depletion in light isotopes (Krummenacher et al., 1962). Atmospheric escape and trapping-at-depth scenarios have been proposed to explain both observations (Ardoin et al., 2022; Broadley et al., 2022; Rzeplinski et al., 2022 and references therein), and are not exclusive. Atmospheric escape models stem from the fact that Xe is the easiest to ionise amongst noble gases and to investigate regarding how this could be triggered by extreme UV radiation of the young Sun if sufficient amount of hydrogen or organic matter were present. However, the main challenge is how to lift the heavy Xe through the atmosphere up to levels where it can be lost (Zahnle *et al.*, 2019). Trapping-at-depth scenarios, in turn, suffer from a lack of knowledge on Xe petrological behaviour. Noble gases partitioning between major minerals and melt is indeed a debated issue, with Xe spanning the largest range amongst noble gases crystal/melt partitioning data (noted as $D_{\text{crystal/melt}}^{\text{Xe}}$), with up to 6 orders of magnitude from 6×10^{-4} to 351 for $D_{\text{olivine/basalt}}^{\text{Xe}}$

(Hiyagon and Ozima, 1986; Broadhurst *et al.*, 1992; Heber *et al.*, 2007).

The published experimental $D_{\text{crystal/melt}}^{\text{Xe}}$ values were obtained from samples brought to high *T*, equilibrated with a noble gas medium either at atmospheric P or ~110 MPa, and quenched to room conditions for chemical analysis. A few experiments were carried out at higher P up to 1.5 GPa (Hiyagon and Ozima, 1986) but with only adsorbed air on starting sample as noble gas source. After correction for eventual melt inclusions in crystals, the very large range of $D_{\mathrm{crystal/melt}}^{\mathrm{Xe}}$ values partly results from the interpretation of bubbles in minerals, *i.e.* whether they should be excluded from measurements or not. Indeed, while noble gas content in melts is homogeneous, such is not the case in minerals, with almost systematic reports of heterogeneous distribution of heavy noble gases, often at the micron or submicron scale (Hiyagon and Ozima, 1986; Broadhurst et al., 1992; Heber et al., 2007). Some data were discarded on this ground, despite sometimes clear elemental fractionation from the original gas (Hiyagon and Ozima, 1986), which is not expected for passively trapped gas. Indeed, Xe was observed to retro-diffuse out of olivine in high P experiments upon T-quenching (Sanloup et al., 2011), an exsolution process that could explain at least part of the bubbles observed on quenched samples. It is therefore very challenging to interpret the heterogeneous distribution of Xe in quenched minerals recovered from experiments.

Another source of controversy arises from the impact of noble gases adsorption on minerals, *i.e.* whether or not it is significant in experiments, and therefore if it should be corrected

^{*} Corresponding author (email: chrystele.sanloup@sorbonne-universite.fr)



^{1.} Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, CNRS, Paris, 75005, France

^{2.} LP2I, UMR5797, Université de Bordeaux, CNRS, Gradignan, 33170, France

^{3.} HPCAT, X-ray Science Division, Argonne National Laboratory, Argonne, 60439, IL, USA

for or not. Step heating experiments show that heavy noble gases are tightly bound in minerals, with largest fractions being released above 1000 °C (Hiyagon and Ozima, 1986), arguing against physical adsorption.

Last but not least, datasets are difficult to compare due to the different compositions used for both melts and crystals (Table 1). For instance, olivine-melt experiment compositions range from synthetic Fe-free forsterite/61 % SiO₂-rich melt (Heber *et al.*, 2007) to natural olivine/basalt (Hiyagon and Ozima, 1986). It is, nonetheless, established that melt composition strongly affects trace element partitioning (Schmidt *et al.*, 2006), with one order of magnitude difference between gabbroic and granitic melts, an effect also expected to be strong for noble gases based on solubility values in melts (Carroll and Stolper, 1993; Schmidt and Keppler, 2002).

Facing these experimental controversies, the peridotitic database shows an enrichment in Xe over other noble gases in xenoliths (Hennecke and Manuel, 1975; Poreda and Farley, 1992; Czuppon *et al.*, 2009). Consistently, natural measurements of Xe mineral/basalt partitioning obtained by analysing parent and partially crystallised magmas (Batiza *et al.*, 1979), or coexisting magma and olivine crystals (Kaneoka *et al.*, 1983), show Xe compatibility with $D_{\text{crystal/basalt}}^{\text{Xe}}$ a few-fold above unity. Natural measurements must, nonetheless, be considered with caution (Carroll and Draper, 1994) due to potential magma degassing processes if minerals and melt did not re-equilibrate, and/or if crystals contain vapour inclusions (Kaneoka *et al.*, 1983), which as for experiments are difficult to interpret.

To circumvent these problems, we have recently developed a new method combining synchrotron X-ray fluorescence and diffraction techniques with large volume presses (Chen *et al.*, 2022). The method was first tested on crystal/felsic melt Xe partitioning, and Xe was found to be moderately incompatible to compatible, with a *T*-dependent behaviour (0.50 ± 0.20 for $D_{\text{plagioclase/melt}}^{\text{Xe}}$ at 1010 °C to 3.46 ± 0.25 for $D_{\text{jadeite/melt}}^{\text{Xe}}$ at 700 °C). This method is applied here to a Paris-Edinburgh press energydispersive set-up, which has the additional advantage of being optimised for the observation of diffuse X-ray scattering signal from melts.

Mineral/Melt Xenon Partitioning Measurements

We measured Xe partition coefficient between olivine and basalt, and between feldspar-clinopyroxene mix and basalt, in order to target Xe petrological behaviour in early Hadean contexts (e.g., magma oceans in planetary embryos) and present day subduction zone contexts respectively. Xenon crystal/ melt partition coefficients were measured by means of in situ synchrotron X-ray diffraction and X-ray fluorescence simultaneously collected on the same spectrum, using an energydispersive set-up and a Paris-Edinburgh press to generate high P-T conditions (Supplementary Information). The starting sample (Supplementary Information) is a synthetic glass relevant for lunar-like magma ocean at the stage of anorthite crystallisation, doped by high P-T synthesis with 0.05 wt. % Xe (Table S-1), i.e. well below Xe solubility in tholeiitic melt (Schmidt and Keppler, 2002) of 0.41 wt. % at 2 GPa to avoid supersaturation, while being high enough for the Xe fluorescence signal to be significantly above noise level. The starting sample is used either pure to mimic planetesimal magma ocean stages or mixed with 10 wt. % labradorite feldspar to get an analogue of high alumina basalts, relevant for present day subduction zone settings. At each targeted P, T was first raised until

recrystallisation, further raised until full remelting, and lowered until crystals grew in equilibrium with melt to ensure chemical equilibrium. The sample was then scanned perpendicularly to the X-ray beam in order to probe either pure melt or crystallised areas. For the olivine/basalt experiments, crystals were efficiently segregated from melt due to their density difference. This was not the case of the pyroxene-feldspar/basalt experiments for which it was not possible to probe only crystals, and the fraction of melt vs. crystals in crystal-rich areas was determined from the X-ray diffraction signal (Supplementary Information). Xenon content in pure melt or crystals was obtained from the Xe K_{α} fluorescence intensity signal in the fully molten sample pattern and the relevant pattern, either pure melt or crystals, at crystal-melt equilibrium (Supplementary Information). If a pure crystal pattern could not be obtained, Xe content in crystals from mixed crystals + melt pattern was obtained using mass-balance calculation from Xe K_{α} fluorescence intensity in crystal-rich area and local melt fraction obtained from X-ray diffraction signal (Eq. S-3).

For basaltic melt in equilibrium with feldspar and pyroxene, Xe was enriched in the melt as seen by the stronger Xe fluorescence signal (Fig. 1) and the derived partition coefficient $(0.16 \pm 0.06; \text{ Table 2})$. Crystal growth partly occurred upon quenching to room T (see microlithic texture of sample in Fig. S-3), hence it is difficult to have a proper estimate of feldspar vs. pyroxene at high *P*-*T* conditions, and oriented crystal growth prevents estimate from in situ energy-dispersive X-ray diffraction data. Nonetheless, due to the low global *D* value, Xe had to be incompatible with both pyroxene and feldspar at our experimental conditions, consistent with the reported T-dependence of D for clinopyroxene/felsic melt (Chen et al., 2022). In contrast, Xe fluorescence signal was not detected in basalt coexisting with olivine (Fig. 1), which implies a lower limit of 80 for $D_{\text{olivine/basalt'}}^{\text{Xe}}$ taking the noise oscillations as a maximum for Xe fluorescence signal in melt. Xenon X-ray fluorescence signal in olivine crystals is strongly affected by quenching *T* at high *P*, with a 2.9 factor decrease in intensity (Fig. 1a), indicating important-although incomplete—Xe exsolution back to room T, consistent with previous observation from in situ X-ray diffraction (Sanloup et al., 2011).

To further constrain Xe concentration in melt coexisting with olivine, pieces of glass recovered from synchrotron experiments and an additional sample synthesised at similar P-T conditions (Supplementary Information) were analysed by noble gas mass spectrometry. From the additional sample, three fragments of glass and two fragments of mostly crystals could be separated, as olivine crystals had sedimented at the bottom of the capsule. Mass spectrometry analyses were done on bulk sample fragments fully melted by laser heating (Supplementary Information), revealing systematic Xe enrichment in olivine-rich fragments compared to glass. Olivine content in olivine-rich fragments is estimated at 83 ± 10 % from analyses of SEM images (Fig. S-3) using ImageJ software. Our reported values of $D_{\text{olivine/basalt'}}^{\text{Xe}}$ 88(22)–302(46) (Table 2), exceed 80 as expected from the lack of Xe X-ray fluorescence signal in the melt. The lower range value was obtained using Xe content in crystals as measured from energy-dispersive X-ray data, and Xe content in glass as measured by mass spectrometry (Table S-2), which is near the 104(16) value obtained on the additional sample using mass spectrometry results only. The upper range corresponds to that value times the intensity ratio between crystals at high *P*-*T* and guenched crystals at high *P* (i.e. 2.9 GPa), to account for Xe exsolution from olivine crystals upon quenching.

2007), step heati glass compositio solubility. Error [ing (Hiyagon and Ozima, 1986; Broadhurst et a n is bulk sample starting composition. Data wh bars on <i>D</i> are given when available; * error ec	<i>I.</i> , 1992). I ere lithiur quals <i>D</i> va	been rounded at annuy, given meet we we way and Data discarded by authors due to contaminatio n borate was added to lower melting <i>T</i> are not lues.	included, as bora	gas. An any used is communed by the modifies melt polymerisation which content te modifies melt polymerisation which content te modifies melt polymerisation which content terms are as a second secon	do Ozima (1986), trols noble gases
Run (ref.)	Thermal treatment (duration @ °C)	P (GPa)	Glass composition (wt. %)	Crystal	Gas composition (mol %)	D ^{Xe} (error)
olivine-melt pa	rtitioning					
V (B1992)	18 d @ 1300	10^{-4}	54SiO ₂ -15Al ₂ O ₃ -14MgO-17CaO	natural forsterite	5Ne-93Ar-1Kr-1Xe	06
RB587 (H2007)	1 h @ 1165 + 3 h @ 1045 + 6 h @ 990	0.1	61SiO ₂ -15Al ₂ O ₃ -23Na ₂ O	$\mathrm{Mg_2SiO_4}$	25He-23Ne-25Ar-22Kr-5Xe	$3.9 \times 10^{-3} - 351$
RB588 (H2007)	1 h @ 1165 + 3 h @ 1045 + 6 h @ 990	0.1	61SiO ₂ -16Al ₂ O ₃ -24Na ₂ O	Mg_2SiO_4	25He-23Ne-25Ar-22Kr-5Xe	$6 \times 10^{-4} - 148$
RB589 (H2007)	1 h @ 1165 + 3 h @ 1045 + 6 h @ 990	0.1	58SiO ₂ -16Al ₂ O ₃ -23Na ₂ O	Mg_2SiO_4	25He-23Ne-25Ar-22Kr-5Xe	0
BH-257 (H1986)	3 h 23 min @ 1370	10^{-4}	48SiO ₂ -15Al ₂ O ₃ -10FeO-15MgO-7CaO-1Na ₂ O	(Mg,Fe) ₂ SiO ₄	11He-1Ne-88Ar-0.3Kr-0.1Xe + CO ₂ -H ₂ (0.5 to 1 ratio)	0.197(0.080)
BH-258 (H1986)	7 h 36 min @ 1370	10^{-4}	48SiO ₂ -15Al ₂ O ₃ -10FeO-15MgO-7CaO-1Na ₂ O	(Mg,Fe) ₂ SiO ₄	11He-1Ne-88Ar-0.3Kr-0.1Xe + CO ₂ -H ₂ (0.5 to 1 ratio)	0.240(0.069)
BH-276 (H1986)	14 h 20 min @ 1350	10^{-4}	48SiO ₂ -15Al ₂ O ₃ -10FeO-15MgO-7CaO-1Na ₂ O	(Mg,Fe) ₂ SiO ₄	115He-1Ne-88Ar-0.3Kr-0.1Xe + CO ₂ -H ₂ (0.5 to 1 ratio)	0.222(0.059)
HPP-1 (H1986)	10 min @ 1350	1.0	48SiO ₂ -15Al ₂ O ₃ -10FeO-15MgO-7CaO-1Na ₂ O	(Mg,Fe) ₂ SiO ₄	air adsorbed on powder	0.14(0.05)
HPP-3 (H1986)	4 h @ 1360	1.5	48SiO ₂ -15Al ₂ O ₃ -10FeO-15MgO-7CaO-1Na ₂ O	$(Mg,Fe)_2SiO_4$	air adsorbed on powder	0.046(0.016)
pyroxene-melt	partitioning					
IV (B1992)	18 d @ 1300	10^{-4}	56SiO ₂ -11Al ₂ O ₃ -15MgO-19CaO	natural diopside	5Ne-93Ar-1Kr-1Xe	3.3
V (B1992)	7 d @ 1332	10^{-4}	56SiO ₂ -11Al ₂ O ₃ -15MgO-19CaO	natural diopside	5Ne-93Ar-1Kr-1Xe	47
VI (B1992)	9 d @ 1332	10^{-4}	56SiO ₂ -11Al ₂ O ₃ -15MgO-19CaO	natural diopside	5Ne-93Ar-1Kr-1Xe	4.0
RB586 (H2007)	0 h 30 min @ 1290 + 1 h @ 1272 + 6 h @ 1200	0.1	65SiO ₂ -14Al ₂ O ₃ -4MgO-8CaO	$(Mg_{x}Ca_{y})SiO_{3}$	25He-23Ne-25Ar-22Kr-5Xe	$0.2-70 \times 10^{-3} *$
HH355 (C2022)	2 h 30 min @ 950 + 3 h 45 min @ 700	1.6	67SiO ₂ -15Al ₂ O ₃ -1CaO-5Na ₂ O	jadeite	Xe	3.58
HH357 (C2022)	4 h 20 min @ 850	1.7	60SiO ₂ -18Al ₂ O ₃ -1MgO-2CaO-8Na ₂ O	omphacite	Xe	2.54
feldspar-melt p	artitioning					
Cell5 (C2022)	6 h 30 min @ 1010	2.0	$63SiO_2-24Al_2O_3-5CaO-8Na_2O$	plagioclase	Xe	0.76

Geochemical Perspectives Letters

Letter



Figure 1 Energy-dispersive X-ray data sets. (Left) Full data sets collected at 10.031°. For each crystal/melt system, data collected at different *T* are vertically spaced for clarity: fully molten sample (orange), partially molten sample (red for molten zone, black for crystalline or crystal-rich zone), and quenched crystals (black dashed). Peaks at 33 keV and 47 keV are MgO diffraction peaks from the cell-assembly. (Right) Zoom on the Xe $K_{\alpha 1}$ and $K_{\alpha 2}$ fluorescence lines (29.4 keV and 29.7 keV). For olivine-melt experiments, data sets in the zoomed panel were collected at 4.0285° to avoid diffraction peaks from crystals overlapping with Xe fluorescence lines.

 Table 2 Run conditions, coexisting phases, crystalline fraction in crystal-rich areas, Xe content in each phase (wt. %), and partitioning coefficients. Note that crystal and melt fractions do not apply to the whole sample but only to the volume probed by the X-ray beam.

 *Mass spectrometry measurement. Values in parentheses are errors on the last reported digits.

Run	P (GPa)	<i>T</i> (°C)	Phases	X _{crystals}	[Xe] ^{crystals} (wt. %)	[Xe] ^{melt} (wt. %)	$D_{ m crystal/melt}^{ m Xe}$
Cell2	2.0	1270	Ol + melt	100(5)	0.145(36)	$1.65(15) \times 10^{-3*}$	88(22)
PC265	1.3	1100	Ol + glass	83(10)	0.015(6)*	$1.5(8) \times 10^{-4*}$	104(16)-302(46)
Cell3	1.2	1120	An + Di + melt	34(4)	0.007(2)	0.044(9)	0.16(6)

Olivine Retains Xe in Magmatic Processes

Clinopyroxene-feldspar/melt data are broadly consistent with the T-trend reported for pyroxene/felsic melt under similar P (Chen et al., 2022), and intermediate within the range of literature values at ambient or near ambient P (Broadhurst et al., 1992; Heber et al., 2007). Olivine/melt data (Fig. 2) confirm the compatible nature of Xe in olivine predicted from ab initio calculations (Crépisson et al., 2018), are similar to ambient P data from Broadhurst et al. (1992), and correspond to the higher range from Heber et al. (2007). The latter study may underestimate $D_{\text{olivine/basalt}}^{Xe}$ as 1) the melt was enriched in silica (Table 1) while Xe solubility increases by a factor of five, for instance, between a MORB and a haplogranite (Leroy et al., 2019), and 2) crystals with bubbles were discarded on the basis of potential contamination while, at least, some of the bubbles are expected to form upon T-quenching, although this effect could be restricted to high P conditions.

Considered together, the present high P-T clinopyroxenefeldspar/melt and olivine/melt data are consistent with the natural reports of bulk peridotite/melt partitioning coefficient a fewfold above unity from oceanic island basalts (Batiza et al., 1979; Kaneoka *et al.*, 1983). The *P* effect on $D_{\text{crystal/melt}}^{\text{Xe}}$ could not be investigated here due to the limited *P*-*T* stability field of the mineralogical parageneses investigated. It further cannot be inferred from the comparison of the present and previous datasets (Fig. S-5) as data are either at ambient or near ambient P (10⁻⁴ and 0.1 GPa) or in a restricted *P*-range between 1.0 and 2.0 GPa. Additionally, the only high P previous dataset for olivine/melt partitioning was obtained with only air adsorbed on samples as a source of noble gases (Hiyagon and Ozima, 1986). Pressure is, nonetheless, expected to be important as Xe retention in silicates is P-induced. Importantly, Xe retention does not extend to lower mantle silicates (Shcheka and Keppler, 2012), consistent with the plume source being depleted in Xe compared to MORB source (Parai, 2022).

As for any element, Xe crystal chemistry controls its partitioning behaviour, and its knowledge is key to understand its



Figure 2 Summary of Xe crystal/melt partition coefficients. Data abbreviations: H1986, Hiyagon and Ozima (1986); B1992, Broadhurst *et al.* (1992); H2007, Heber *et al.* (2007); C2022, Chen *et al.* (2022); PC265, Cell2, and Cell3 are data from this study (Table 2). Empty symbols indicate room *P* data; filled symbols indicate data collected between 1.0 and 2.0 GPa (*cf.* Table 1). Note that Heber *et al.* (2007) discarded all values above unity due to the observation of gas bubbles in crystals, while at least some might form from exsolution upon quenching. Natural rocks dataset: residual rock/basalt partition coefficients from Batiza *et al.* (1979).

repartition in planetary envelopes. In magmas, noble gases enter the ring structure of silicate melts (Carroll and Stolper, 1993), eventually leading to oxidation in the case of Xe in compressed silica-rich melt (Leroy et al., 2019). In minerals, the tightly bound nature of Xe leads to the suggestion that either interstitial sites or crystal vacancies are possible sites for the Xe atoms (Hiyagon and Ozima, 1986). Theoretical calculations have shown that Xe can chemically bond to oxygen in quartz (Probert, 2010; Crépisson et al., 2019) and olivine (Crépisson et al., 2018) under modest P by substituting a Si atom. This precludes the use of mineral/ melt partitioning models considering Xe as a 'zero'-charge species (Brooker et al., 2003). The radius of chemically bonded Xe is, indeed, much smaller than that of inert Xe, with three oxygen atoms located at 2.0 Å in a planar configuration in olivine (Crépisson et al., 2018), and two nearest oxygen atoms at 2.0 Å, and two further ones at 2.3 Å in quartz (Crépisson et al., 2019). Xenon crystal chemistry has not been reported for pyroxene nor feldspar but for the latter it might be similar to that in quartz, both being tectosilicates. The contrasting $D_{\text{crystal/melt}}^{\text{Xe}}$ values between olivine/basalt and pyroxene-feldspar/basalt may relate to the different local environments of Xe in these minerals.

Over the course of Earth's history, Xe should have been strongly retained in olivines crystallising from magma oceans, and in olivine-rich residues in present day mantle partial melting processes. Preferential release to the atmosphere is instead expected from high T (>1000 °C) crustal processes, turning to a moderate retention in pyroxenes and feldspars equilibrated with lower T melts such as evolved hydrous magmas in continental crust and arc contexts (Chen *et al.*, 2022). The petrological behaviour of Xe hence supports the trapping-at-depth scenario (Rzeplinski *et al.*, 2022), whereby a succession of collisions between pre-planetary embryos led to the depletion in terrestrial and Martian Xe light isotopes due to Xe trapping and oxidation in crystallising magma oceans, while over 99 % (Harper and Jacobsen, 1996) of the initial budget was expelled from growing planetesimals by exsolution from melt at low P in convecting magma oceans followed by atmospheric losses on a few Myr timescale. The late veneer chondritic input to the atmosphere followed by partial-only Xe degassing concomitantly with the emplacement of the continental crust led to the rising Kr/Xe ratio and progressively heavier Xe observed in Archean atmospheric samples (Broadley et al., 2022) until the late veneer got overprinted, while lighter Xe in the mantle (Peron and Moreira, 2018) would result from mixing mass fractionated Xe with subducted Archean atmospheric Xe. This Archean evolution is not observed on Mars where such events did not occur. That the retention of Xe differs in minerals while its impact on isotopic fractionating is similar (Rzeplinski et al., 2022) implies that Xe elemental and isotopic evolution cannot be modelled by the same Rayleigh distillation law. Indeed, Rayleigh-predicted Kr/Xe ratios for the Archean atmosphere disagree (Broadley et al., 2022), a mismatch attributed to variable Xe loss over time which is challenging to reconcile with a continuous isotopic evolution.

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Additional Information

Supplementary Information accompanies this letter at https:// www.geochemicalperspectivesletters.org/article2413.



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Xenon compatibility in magmatic processes: Hadean to current contexts

Q. Chen, C. Sanloup, D. Horlait, G. Shen

Supplementary Information

The Supplementary Information includes:

- ➤ Methods
- > Tables S-1 and S-2
- > Figures S-1 to S-5
- ➢ MS Datasheets S-1 to S-7
- > Supplementary Information References

Methods

Sample preparation

For olivine/melt partitioning experiments, starting glass (Table S-1) was prepared from reagent grade oxides and carbonates powders to reproduce the composition of lunar magma ocean at the stage of anorthite crystallisation (Sakai *et al.*, 2014). Powders were first ground and decarbonated by slowly heating in a platinum crucible in an atmospheric furnace from room temperature to 1000 °C, run for 10 hours, molten at 1500 °C for 1 hour, and then quenched in water. Recovered glass was crushed into powder again and remolten twice to ensure homogeneity. Xenon doping was done using a gas loading device (Boettcher *et al.*, 1989) to introduce Xe in a platinum capsule previously filled to one third with crushed glass, and brought to 1610 °C and 2.2 GPa for 40 minutes with a piston cylinder press (run PC202, 'Xe-doped glass' in Table S-1). For mass spectrometry analyses, an additional sample was synthesised (run PC265) using as starting composition a previously Xe-doped basaltic glass synthesised similarly to run PC202, recovered, loaded in a new Pt capsule, and brought to 1.3 GPa and 1100 °C for 3 hours to reach the basalt-olivine stability field. PC265 sample experienced the most massive Fe loss, due to the two successive loadings and piston-cylinder runs using two different Pt capsules. For clinopyroxene-feldspar/melt partitioning experiments, the starting sample was obtained from mixing 90 wt. % of previously synthesised glass with 10 wt. % feldspar (labradorite from Spectrum Mine, Plush, Lake Co., Oregon, courtesy of Marie Baïsset).

In situ partitioning measurements

In situ synchrotron experiments were conducted on beamline 16-BM-B at the Advanced Photon Source (Chicago, U.S.A.). High *P-T* conditions were generated using a Paris-Edinburgh press, with cell-assembly



described in Yamada et al. (2011). An energy-dispersive X-ray set-up allowed the simultaneous collection of the diffraction and fluorescence signals on coexisting crystals and melt. To constrain the X-ray path length through the sample and preserve the sample cylindrical geometry, diamond capsules (inner diameter of 750 µm) were used and sealed under P by platinum-rhodium caps. MgO cylinder surrounding the graphite heater was modified with two boron-epoxy windows to reduce X-ray absorption for both the incident and diffracted X-rays. Temperature was calibrated from power-T curve calibrated against melting temperatures of salts (Kono et al., 2014), and P was calculated from the cell volume of MgO (Kono et al., 2010). Uncertainties on P and T are respectively 0.3 GPa and 80 °C. The design of the cell-assembly insures remarkable stability under high P-T conditions and a large vertical access to the sample throughout the experiment. At each P-Tcondition, an X-ray radiograph image of the sample was recorded (Fig. S-1), attesting that the whole sample could be probed through the anvil gap. Energy dispersive X-ray (EDX) data were collected on a Ge solid-state detector with slit size defining the X-ray beam of either $50 \times 100 \ \mu\text{m}^2$ or $100 \times 100 \ \mu\text{m}^2$, with collection time of 1800 s to 6700 s to optimise the signal to noise ratio for the Xe fluorescence peaks. EDX data were collected with the scattering angle $(2-\theta)$ at $10.0310 \pm 0.0007^{\circ}$, or at $4.0285 \pm 0.0005^{\circ}$ if overlap of Xe fluorescence and Bragg diffraction peaks occurred at the higher 2- θ value. EDX data were processed by normalising intensities with live time, and slits size if different between datasets. Due to the lack of information on crystal preferential orientation using EDX, it is not possible to calculate crystal fraction from crystalline Bragg peaks area. Instead, EDX spectra collected on MgO at the same P-T conditions as crystal-melt equilibrium were taken as background intensity to calculate crystals vs. melt fraction from the intensity ratio between baselines from crystal-rich and melt patterns after background subtraction (Fig. S-2). In the case of Cell2, MgO and crystalline spectra have an overlapping baseline, indicating a melt content less than noise, *i.e.* less than 5 %.

Xenon concentrations were calculated from Xe K_a X-ray fluorescence line using the method described in Chen *et al.* (2022), where the absolute intensity of the fluorescence signal, I_i , depends on the following factors (Simabuco and Nascimento Filho, 1994): (1) beam intensity I_i^0 , (2) Xe concentration in the sample [Xe]_i, (3) average density ρ_i , (4) volume of the sample probed by the X-ray beam path V_i , (5) absorption by the sample and the surrounding cell-assembly A, and (6) detector sensitivity S as:

$$[Xe]_i = \frac{I_i}{I_i^0 \times \rho_i \times V_i \times 10^{-A} \times S}$$
(S-1)

The factors I_i^0 , A, and S are identical between crystal-rich and melt patterns. For both synchrotron runs, the sample was first fully molten at the targeted P, hence cell-assembly deformation between fully molten state and slightly cooled mineral-melt equilibrium state can be neglected, and Equation S-1 can be simplified to:

$$[Xe]_i = [Xe]_{\text{fullmelt}} \times \frac{\Lambda_i}{\Lambda_{\text{fullmelt}}} \times \frac{\rho_{\text{fullmelt}}}{\rho_i}$$
(S-2)

with $[Xe]_{fullmelt}$ taken as the starting glass Xe content, and Λ the Xe K_a fluorescence peak area. Density of crystals and melts were calculated from (1) the Murnaghan equation of state and the thermal expansion for anorthite (Tribaudino *et al.*, 2010; Angel, 2004), (2) 3rd order Birch-Murnaghan equation of state for olivine (Liu and Li, 2006), (3) the high-*T* Birch-Murnaghan equation of state of diopside (Zhao *et al.*, 1998), and (4) from the 3rd order Birch-Murnaghan equation of state of mantle melts (Agee and Walker, 1988) and the compositional dependence from the ideal mixing model (Lange and Carmichael, 1987).

For datasets containing a mixture of melt and crystals, Xe weight fraction in crystals can be obtained from mass balance calculations:

$$[Xe]_{c} = \frac{[Xe]_{i} - x_{i,m}[Xe]_{melt}}{(1 - x_{i,m})}$$
(S-3)

where $x_{i,m}$ is the melt fraction in pattern *i*, and [Xe]_{melt} is taken from the coexisting pure melt pattern.

Textural, chemical, and mineralogical analyses

Recovered sample images were obtained using a Zeiss Ultra 55 field emission scanning electron microscope (SEM), with a working distance of 7.5 mm and a voltage of 20 kV for detection of Xe. Note that samples recovered from present synchrotron experiments are all bubble free at the SEM scale (Fig. S-3). A few Xe submicron bubbles are observed inside olivine crystals from the additional basalt/olivine sample, although rarely. The major elements (Table S-1) of starting glass and recovered samples were determined using a Cameca SX-FIVE electron probe microanalyser (EPMA) on the Camparis platform at Sorbonne University. Accelerating voltage was set to 15 kV, with 5 nA beam current for Na, Ca, Al, Si and 40 nA for Xe. Note that in order to recover the samples from Paris-Edinburgh press experiments, diamond capsules had to be cracked and polished down. Xenon content in the starting glass was measured by EPMA using Xe calibration established following the procedure developed by Montana *et al.* (1993) by measuring the counts for the neighbouring elements, I (CuI) and Cs (CsCI).

Raman spectra were recorded on a JobinYvon Horiba HR460 spectrometer using a single-grating monochromator with 1500 gratings/mm and an argon laser (514.5 nm wavelength) to confirm the mineralogy of recovered samples (Fig. S-4) as obtained from EPMA analyses.

Mass spectrometry analyses

Xenon content on recovered glass pieces from Cell2, and both crystal-rich and glass pieces from run PC265, was measured by mass-spectrometry (Table S-2). Mass spectrometry (MS) measurements were done at the PIAGARA platform (LP2i-Bordeaux). The samples were beforehand weighted using a CAHN/Ventron 21 automatic electro-balance after performing the mandatory daily calibration. Although this electro-balance is precise down to 0.1 μ g (for sample below 2 mg), a $\pm 1 \mu$ g error is considered to take into account sample contamination or conversely surface erosion by handling.

The MS employed for the analyses is originally a model 1202 of V. G. Micromass 12 (magnetic sector, 60° deflection, and 12 cm radius instrument), incorporating in a small interior volume and customised with a Nier-type source (from a VG3000) and a Cu-Be electron multiplier detector for quantification (integration counting mode). Each sample was placed in an ultra-high vacuum chamber (below 10^{-8} mbar) and a laser was focused on the base of the sample holder (a Mo crucible, previously annealed at circa 2000 °C under vacuum to eliminate any possible Xe contamination). Description of the laser heating setup is reported in (Horlait et al., 2021). A light laser power was first applied for few minutes to bring the sample and base holder at 50-100 °C in order to check for the presence of atmospheric contamination (physical sorption). For all three measured samples (seven fragments in total), no Xe was detected above the usual blank (few 10⁵ of each major Xe isotope) after this pre-heating treatment. The sample fragment was then melted by progressively increasing the laser power. A camera is used to monitor sample evolution and the latter is considered melted once its original form changed to a round shape. After the visual observation of melting, the laser power was still conservatively increased by ~ 10 % and let steady for a few tens of seconds. For the tiniest samples (1 or 4 μ g, see Table S-2), laser power obtained when melting larger sample fragments were applied. The evolved gas was treated by hot metallic powders to trap non-noble gases species and thus let only Xe into the MS setup (Horlait et al., 2021). After a rapid estimation of Xe content by MS with a tiny fraction of the gas released from melted samples, the remaining fraction was spiked with a known amount of a monoisotopic ¹³¹Xe gas before introduction in the MS. Xenon content from the sample was then deduced from the ${}^{i}Xe/{}^{131}Xe$ intensity ratios measured by MS. This approach allows reducing MS measurements errors to circa 5 % (main sources of errors stem from uncertainties of pipes volumes and spike ¹³¹Xe content). As required the FileMaker sheet compiling raw MS measurements are given in MS Datasheets S-1 to S-7. Individual [Xe] values determined by MS and electro-balance measurements are listed in Table S-2.



Supplementary Tables

Table S-1Chemical analyses of starting and quenched samples (wt. %). Note that Fe loss may have occurred at
two stages, during Xe-doping using platinum capsules in piston-cylinder press experiments which is particularly strong
for PC265 due to the successive use of two Pt capsules, and during synchrotron experiments due to Pt-Rh caps used to
seal diamond capsules.

Sample	Na ₂ O	FeO	CaO	MgO	SiO ₂	Al ₂ O ₃	Totals
Xe-doped glass	-	12.54	13.47	10.44	45.14	17.24	99.22
		(0.25)	(0.26)	(0.18)	(0.59)	(0.16)	(1.15)
Cell2 quenched glass	-	4.88	15.27	13.07	49.08	18.79	101.31
		(0.19)	(0.28)	(0.22)	(0.52)	(0.26)	(0.73)
Cell2 olivine	-	8.81	0.35	51.12	42.26	0.10	102.75
		(0.87)	(0.06)	(1.16)	(0.45)	(0.05)	(1.1)
PC265 quenched glass	-	3.40	13.77	9.82	48.84	21.21	97.21
		(0.11)	(0.18)	(0.12)	(0.35)	(0.28)	(0.66)
PC265 olivine	-	0.42	0.45	55.83	44.09	0.44	101.41
		(0.61)	(0.29)	(0.96)	(0.66)	(0.35)	(0.71)
Cell3 quenched glass	0.95	0.28	14.52	12.16	49.26	19.62)	96.91
	(0.04)	(0.04)	(0.16)	(0.52)	(0.60)	(0.51)	(0.72)
Cell3 anorthite	1.87	0.17	17.30	0.93	48.77	30.47	99.65
	(0.11)	(0.03)	(0.63)	(0.06)	(0.28)	(1.97)	(0.78)
Cell3 diopside	0.18	0.42	14.96	26.91	53.32	9.29	105.34
	(0.04)	(0.36)	(0.97)	(1.13)	(0.090)	(1.15)	(0.41)

Table S-2 Mass spectrometry analyses. Errors on the Xe contents (from the variance of individual measurements) are given in brackets and refer to the last digit(s) of the corresponding value. Weighted averaging of Xe contents were done by pondering each value by the inverse square of its relative error. To better reflect that dispersion of results from a fragment to another presumably comes from samples heterogeneity rather than from Xe content measurements uncertainties, the errors in the last column are calculated from the variance against the average value of the individual Xe content values.

Analysis	Phase	Weight (µg)	Xe content (wt. %)		
Cell2, piece 1	glass	57	$1.84(7) \times 10^{-3}$		
Cell2, piece 2	glass	65	$1.42(6) \times 10^{-3}$		
Cell2	glass average		1.65(15) × 10 ^{−3}		
PC265, piece 1	glass	16	$8.9(4) imes 10^{-5}$		
PC265, piece 2	glass	1	9.4(4.7) × 10 ⁻⁵		
PC265, piece 3	glass	18.8	$3.7(2) \times 10^{-4}$		
PC265	glass average		$1.5(8) \times 10^{-4}$		
PC265, piece 4	olivine-rich	4	$2.0(6) imes 10^{-2}$		
PC265, piece 5	olivine-rich	4	$4.8(1.5) \times 10^{-3}$		
PC265	olivine-rich average		1.3(5) × 10 ⁻²		



Supplementary Figures



Figure S-1 X-ray radiographs taken at crystals-melt equilibrium and after quenching to room T at high P. (a) olivine/melt experiment (Cell2), (b) pyroxene-feldspar/melt experiment (Cell3). Sample width: 750 μ m. Thin darker zones on radiographs are Pt bits that fell of the Pt capsule upon retrieving the starting Xe-doped glass.





Figure S-2 EDX data collected at 10.031° on anorthite + diopside/melt equilibrium at 1.2 GPa and $1120^{\circ}C$ (Cell3), along with MgO dataset collected at the same *P*-*T* conditions, and taken as background intensity to calculate crystals *vs*. melt fraction (34(4) % crystals for this dataset) from the intensity ratio between baselines from crystal-rich and melt patterns after background subtraction.



Figure S-3 SEM images of quenched samples. Top left: recovered sample piece from the olivine/melt experiment (Cell2) with two visible olivine crystals. Top right: whole recovered sample from the pyroxene-feldspar/melt experiment (Cell3), with mostly small size crystals and a fully glassy zone on the left hand side; bright zones are Pt bits that fell of the Pt capsule used to synthesise the starting Xe-doped glass. Bottom: sample slices from the olivine/melt additional experiment (PC265) used for mass-spectrometry analyses (pure glass on the left and mostly olivine crystals on the right).



Figure S-4 Raman spectra collected on recovered samples from Cell3 and PC265. Spectra from RRUFF database (Lafuente *et al.*, 2016) are shown for comparison and identification of diopside and anorthite.



Figure S-5 Xenon crystal/melt partition coefficients as a function of pressure (left, pyroxene-feldspar/melt; right, olivine/melt). Data abbreviations: H1986, Hiyagon and Ozima (1986); B1992, Broadhurst *et al.* (1992); H2007, Heber *et al.* (2007); C2022, Chen *et al.* (2022); PC265, Cell2, and Cell3 are data from this study (Table 2). Note that Heber *et al.* (2007) discarded all values above unity due to the observation of gas bubbles in crystals.



SI-10





Supplementary MS datasheets

Datasheet S-2 MS datasheet for sample "Cell2, piece 2" (see Table S-2). For details, refer to annotated Datasheet S-1 and its caption.



Datasheet S-3 MS datasheet for sample "PC265, piece 4" (see Table S-2). For details, refer to annotated Datasheet S-1 and its caption.

menu Liste_sample	e KryXe G	Qi PC265 cryst1 KryXe Qi PC265 cryst1 Xe									Xe			KryX	e Qi PC265
1) sample _da	ateID 14/0	4/2022				_propi	rioID	toto		<u>_</u>		_NomCompte toto		PC2	65 cryst1;Xe;
2)Etalon								R	Gnle					·	-
_pipetteID pipE1	ordrelD 56	_refID 131	pip) pipS	lk td	185.24 185.71	0.98 0.00]							
NomEtalonRef	pipE_131			cRefN (185.2	E8at) 4 0.98										
3)Dilution Nom	FracSampIn	Dil [Bg/B2	6ghsH16p					: 0.01669±0	.00012		-
	NomFra	:Pip					ft					: <u>1.00000</u> ±0	.00000		
Spectre:	NomFra	cDil [B23/B25g	hsX1P1PE	12				: 0.15950 ±	0.00245		
IDil : 11.000 ± 0.010	masse Rdil ±	12	4 126	128	129 0.52000 0.05000	130	131 1.00000 0.00100	132 0.52500 0.05000	134	136					
	t t	0.00	2000 0.00		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000					
5) Calculs	masse	12	4 126	128	129	130	131	132	134	136	1				-
	c_Rap ±		?	? ?	0.7162	0.0000	?	0.7072	0.000	0.000)				
	c_Choix				1			1							
	NSa (E	ample ¹ 8at)	31	7 896.194 917.36	40 72	N	samp = (2 mes ±	0.7115 0.0824	i4)≛N 1	pip(
	Si E·	ens 13 -17A/at	31	0.21 0.01	75 11	cR	ap=(Rdil-Rp amp=cRap*	bip)/(Rsam) Npip	p-Rdil)						

Datasheet S-4 MS datasheet for sample "PC265, piece 5" (see Table S-2). For details, refer to annotated Datasheet S-1 and its caption.

menu Liste_sample	KryXe C	i PC265	cryst2	KryXe	Qi PC2	65 cry	/st2 4µg				Xe			KryXe Qi PC265	
1) sample _da	teID 5/05	5/2022				_prop	orioID	toto		9		_NomCompte	0	PC265 cryst2 4µg;X	e;
2)Etalon								R	qGnle						
_pipetteID _o pipE1	59	_refID 131	pipNk pipStd		185.01 0.00	0.98 0.00									
NomEtalonRef	pipE_131			cRefN (E 185.01	8at) 0.98										
3)Dilution NomF	- racSamplı	nDil				H	13/H16p					0.14845±	0.00039		
	NomFra	cPip					ft					: <u>1.00000</u> ±	0.00000		
Spectre:	NomFra	cDil			E	32/B26gh	sH13X1P1P	E12				: 0.03606 ±	0.00047		
IDil : 6.000	masse	124	126	128	129	130	131	132	134	136]				
± 0.010	Rdil ±				0.75000		0.10000	0.76100	0.29100						
	Rpip	0.00000	0.00000	0.00000	0.00000	0.0000	0 1.00000	0.00000	0.00000	0.00000					
	±		0.00000	0.00000	0.00000	0.0000	0.00000	0.00000	0.00000	0.00000					
5) Calculs											,				
ey culculo	masse	9 124	126	128	129	130	131	132	134	136					
	c_Rap ±		1 1 2 2	?	0.0507	0.000	9 1 ? ?	0.0249	0.2444	0.0000					
	c_Choix				1			1	1		1				
	NS:	ample 131 8at)		1 874.442	4	[Nsamp = (3 mes ³	1.5040 0.0222)7)*Np	ip(
	E	-17A/at		0.359 0.006	0	CF N:	Rap=(Rdil-R¢ samp=cRap*	oip)/(Rsam Npip	p-Rdil)						

Datasheet S-5 MS datasheet for sample "PC265, piece 1" (see Table S-2). For details, refer to annotated Datasheet S-1 and its caption.

menu Liste_sample	e KryXe Q	i PC26	5 glass 3	KryXe	Qi PC2	65 gla	ss 3 16µ	ıg			Xe				Kry)	(e Qi PC265 glass
1) sampleda	ateID 4/05/	2022				_propr	rioID	toto		2		_NomCor	npte toto] PC2	65 glass 3 16µg;
2)Etalon								R	qGnle							-
_pipetteID _ pipE1	ordreID 58	_refID 131	pipNk pipStd		185.09 6 885.33	0.98 0.00										
NomEtalonRef	pipE_131			cRefN (E 185.09	8at) 0.98											
3)Dilution Nom	FracSampIn	Dii [B25g	hsX1P1/E	326ghsX1P	1H16p				: 0.416	45± 0.00	0171		-
	NomFrac	Pip					ft					: 1.000	00±0.00	0000		
Spectre: 10278Xe	NomFrac	:Dil [B23/B25g	jhsX1P1PE	12] : 0.159	950 ±0.0	0245		
IDil : <u>3.450</u> ± 0.010	masse Rdil	124	126	128	129 0.30400	130	131 1.00000	132 0.29500	134 0.11500	136						
	Rpip ±	0.00	000 0.00000 ? 0.00000	0.00000 0.00000	0.00000	0.00000 0.00000	1.00000	0.00000	0.00000	0.00000						
5) Calculs	masse	124	126	128	129	130	131	132	134	136						-
	c_Rap ±		<u>s</u> s s	?	0.3227 0.1404	0.0000 ?	?	0.3034 0.1340	0.3054 0.3466	0.0000						
	C_CHOIX															
	NSa (E	imple 1: 8at)	31	138.6884 41.5052	2	N:	samp=(3 mes =	0.3120 ± 0.0933	16)*Np 7	pip(
	Se E-	ens 13 17A/at	1	0.0891 0.0065	5	cRa Nsa	ap=(Rdil-Rp amp=cRap*	oip)/(Rsam Npip	p-Rdil)	_						

Datasheet S-6 MS datasheet for sample "PC265, piece 2" (see Table S-2). For details, refer to annotated Datasheet S-1 and its caption.



Datasheet S-7 MS datasheet for sample "PC265, piece 3" (see Table S-2). For details, refer to annotated Datasheet S-1 and its caption.

menu Liste_sample	Qi PC265	;		Qi PC2	265 18,8	Bug							Qi PC265;Qi PC265
1) sampledate	eID 23/05	/2023]			_propr	rioID	toto		9	_NomCompte	0	18,8ug,,
2)Etalon								R	qGnle				
_pipetteID _or pipE1	67	refID 131	pipNk pipStd		184.40 0.00	0.97 0.00		(E8at) (E8at)					
NomEtalonRef	pipD1_m_{	32		cRefN (E 184.40	8at) 0.97		(E8at)						
3)Dilution NomFr	ac Sampini	Dil			B35	ofghrs/B15	ifghrsX12H	2H67			: 0.29944	0.00240	
	NomFrac	Pip					ft				: <u>1.00000</u> ±(0.00000	
Spectre:	NomFrac	Dil 🗌				B12/B	15fghrsxy				:	0.00137	
IDII : 87.400 nA ± 0.200	masse Rdil * Rpip ±	0.00000	126 0.00000 0.00000	128 0.04942 0.00055 0.00000 0.00000	129 0.66390 0.00230 0.00000 0.00000	130 0.09759 0.00076 0.00000 0.00000	131 1.00000 1.00000 0.00000	132 0.65980 0.00300 0.00000 0.00000	134 0.25597 0.00160 0.00000 0.00000	136 0.21720 0.00130 0.00000 0.00000			
5) Calculs	masse c_Rap ± c_Choix	124 ? ?	126 ? ?	128 1.2060 0.0296	129 1.1403 0.0085 1	130 1.0359 0.0164	131 ? ? 1	132 1.0859 0.0103 1	134 1.0863 0.0142 1	136 1.0844 0.0135 1			
	NSar (E8 Ser E-1	nple 131 at) ns 131 17A/at		682.4361 10.5708 1.7806 0.0246	3	Ri cRa Nsa	samp = (5 mes [:] ap=(Rdil-Rj amp=cRap'	1.108; ± 0.0134 Dip)/(Rsam	20) * Np 18) P-Rdil)	ip(



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