Noble gases in magma ocean

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Study context

- Study the magma ocean during early Earth
- Specifically the behaviour of noble gases in the molten magma
- Magma Ocean = bulk silicate Earth(McDonough and Sun 1995) :

Oxide	Na_2O	FeO	CaO	Al_2O_3	MgO	SiO_2
mol%	0.8	6.5	3.2	2.4	48.4	38.7

- We call this theoretical rock pyrolite
- Ab Initio Molecular Dynamics using VASP software

Study outline

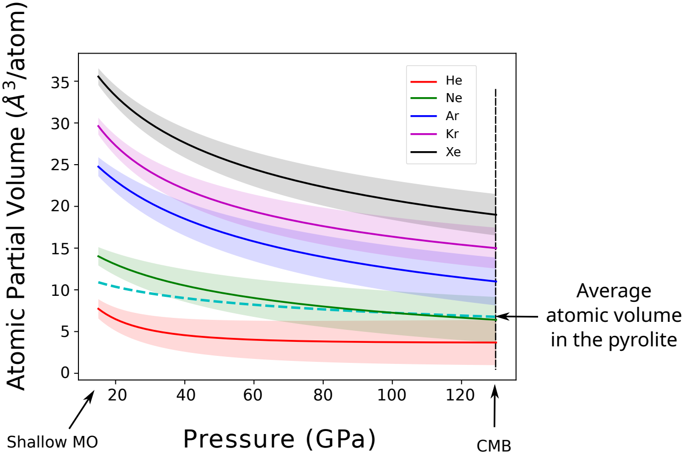
We look at three different physical properties :

- Partial molar volume using the equation of state
- Diffusion using the Mean Square Displacement
- Xe-O bonding using ELF, Bader charges and lifetime of cluster

Partial molar volume in the melt

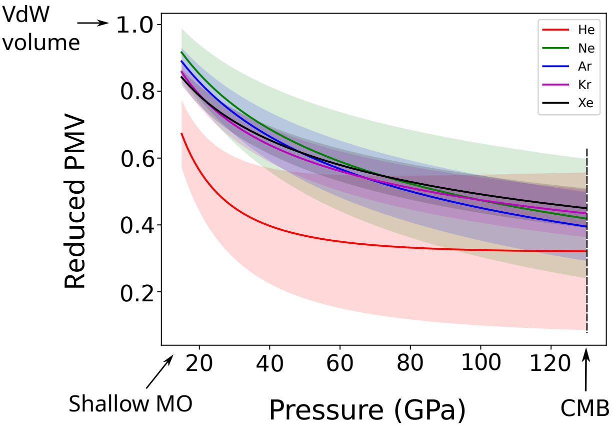
T=5000 K

$$V_{N.G}(P)=V_{pyr+N.G.}(P) - V_{pyr}(P)$$

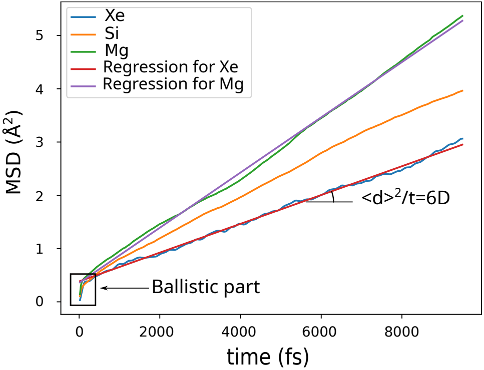


Reduced partial molar volume

T=5000 K

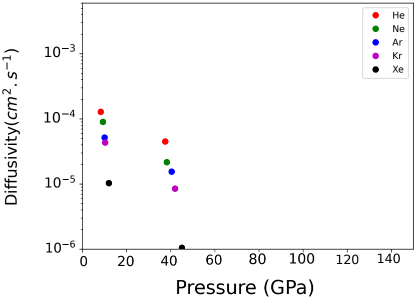


Mean Square Displacement and diffusivity

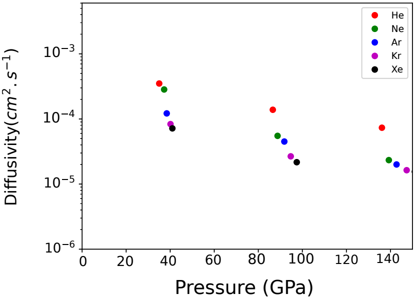


90 GPa and 4000 K

Diffusion Coefficient

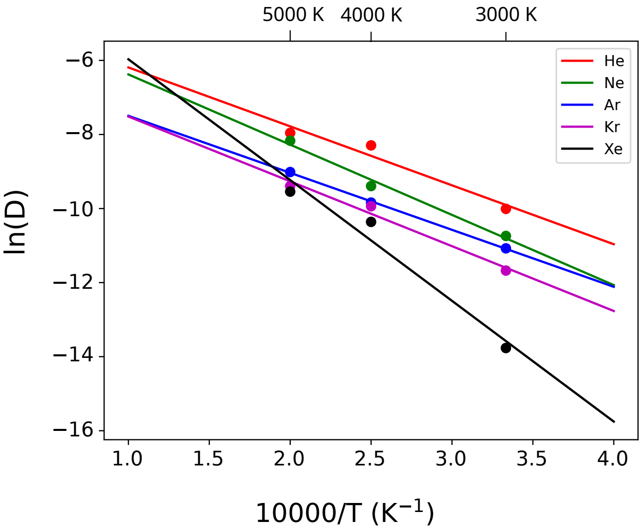


T= 3000 K

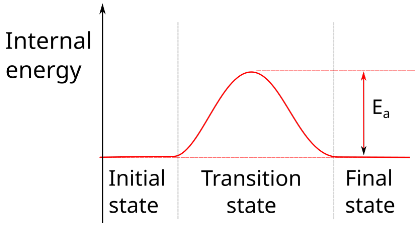


T= 5000 K

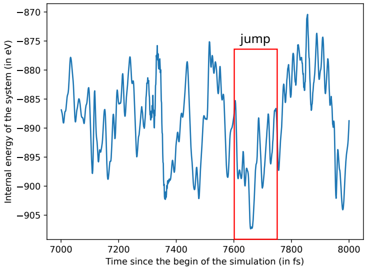
Arrhenius law at 40 GPa



Discussion about the activation energy



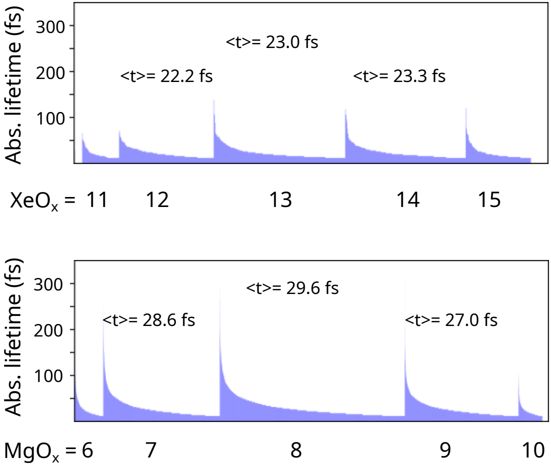
Theoretical energy landscape



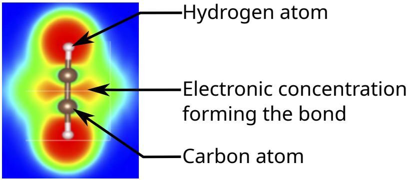
Observed energy landscape

Life time of cluster

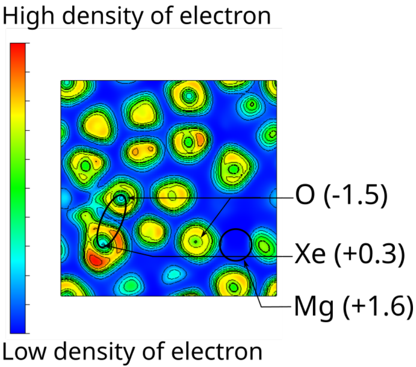
T= 5000 K, P= 120 GPa



Electron localisation function



ELF for covalent bonding (Koumpouras 2020)



Observed ELF for the XeO interaction

Take home message

- Partial molar volume of heavy noble gases converge to the same behaviour while Helium follow a different pattern
- Diffusivity of heavy noble gases converge to the same value at extreme condition while Helium diffuses faster
- The activation energy seems to be a macroscopic quantity which is not related to any observable microscopic effect (no energy variation when the noble gases move)
- There is no evidence of chemical bonding between Xenon and Oxygen in magma ocean (no covalent or ionic bonding)