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Effect of MgO content on noble gas solubility in primitive mantle silicate melts: Insights from molecular dynamics

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Understanding the origin of noble gases in the Earth's mantle remains a major challenge in planetary geochemistry. A widely discussed hypothesis proposes that these elements were incorporated into the Earth's interior through dissolution of a primordial atmosphere into a global magma ocean during the earliest stages of planetary evolution. In this framework, noble gas solubility in silicate melts plays a key role in regulating their storage within the magma ocean and controlling the efficiency of their degassing during melt-atmosphere exchange. Reliable estimates of noble gas solubility in primitive mantle compositions are therefore essential for evaluating the extent of early Earth ingassing. Experimental studies have investigated noble gas solubility in mafic to moderately ultramafic melts, generally limited to compositions containing up to ~21 wt.% MgO [1]. However, the primitive mantle is commonly represented by a pyrolitic composition characterized by substantially higher MgO contents (~37–40 wt.%; [2]), which remains experimentally challenging to maintain under fully molten conditions. As a result, current solubility models for primitive mantle melts largely rely on extrapolations from less magnesian systems. Here, we use classical molecular dynamics simulations combined with the Widom test-particle insertion method to investigate noble gas solubility in MgO-rich silicate melts. The effect of MgO content is explored using compositionally controlled melts with constant SiO_2 (~45 wt.%) and variable MgO enrichment. Solubilities of He, Ne, Ar, Kr, and Xe are quantified at temperatures and pressures representative of an exposed magma ocean. The resulting dataset provides new constraints on the influence of melt composition on noble gas incorporation and assesses whether extrapolations from basaltic compositions adequately capture solubility systematics in primitive mantle melts.

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[2] Lyubetskaya, T., & Korenaga, J. (2007). Chemical composition of Earth's primitive mantle and its variance: 1. Method and results. *Journal of Geophysical Research: Solid Earth*, *112*(B3).