

# **$^{40}\text{Ar}$ Closure Dynamics in Mantle Phlogopite: Theoretical constraints on Pressure Effects.**

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Phlogopite is a common constituent of K/Mg–metasomatized rocks. It is particularly abundant in kimberlite, either as groundmass crystallites formed at depth in the kimberlite melt proper or as megacrysts included in mantle xenoliths entrained during the kimberlite ascent. Due to its high K content, it is an ideal candidate for  $^{40}\text{Ar}/^{39}\text{Ar}$  dating of kimberlite-forming and mantle metasomatism processes, as well as for tracing the evolution of the underlying crust and mantle. Previous studies showed that  $^{40}\text{Ar}/^{39}\text{Ar}$  ages of phlogopite in mantle xenoliths are significantly older than the inferred emplacement age of the kimberlite host. This has been often ascribed to the presence of excess  $^{40}\text{Ar}$ , the main argument being that in situ radiogenic argon cannot be retained within the phlogopite lattice at temperatures significantly above the conventionally determined closure temperatures of argon in this mineral (~480 °C). However, while argon diffusion studies mainly focused on determining the dependence of  $^{40}\text{Ar}$  to temperature, much is unknown regarding its behavior at ultra-high pressure conditions. Existing data in this connection are scanty and contradictory. In this work, we reevaluate the  $^{40}\text{Ar}$  diffusivity in phlogopite and its dependence to both temperature and pressure. To circumvent the problem of mineral instability during laboratory experiments and the potential interference of microstructural defects, we investigate the diffusion process at the atomic scale, by combining Classical Molecular Dynamics simulations with the Transition State Theory. Our results reveal  $^{40}\text{Ar}$  diffusion kinetics several orders of magnitude slower than existing estimates, with a significant effect of pressure that allows preservation of radiogenic  $^{40}\text{Ar}$  in the phlogopite lattice even after a long (Gyrs) residence at mantle P-T conditions. This suggests that phlogopite in mantle xenoliths can yield ages that approximate the time of mantle metasomatism.