Geochemical and geophysical constraints on the nature of mantle convection

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We reconcile the seismic and geochemical observations for slab subduction into the lower mantle with noble gas requirements for a relatively undegassed lower mantle, such as the Earth's ^{40}Ar budget [1]. Using geochemical reservoir modelling that allows for mass flux between upper and lower mantle, we show that recycling and mixing of slabs devoid of noble gases can preserve significant amounts volatiles in the processed and depleted lower mantle. The Earth's budget of radioactive elements (U, Th, K), the difference in ^{3}He/^{4}He and ^{143}Nd/^{144}Nd ratios between mid-ocean ridge basalts and ocean island basalts (OIBs), as well as the high concentrations of ^{3}He and ^{40}Ar in the mantle source of OIBs can be explained self-consistently if ~50% of slabs subduct into the lower mantle, with the rest re-circulating in the upper mantle. This results in a mass flux across the 670 km discontinuity that is equivalent to one lower mantle mass over 4.5 Ga. Hence, to preserve the primitive noble gas signatures and balance the budget of the heat producing elements, we find no need for hidden reservoirs, or convective isolation of the lower mantle for any length of time.

Our findings on the relative rates of plate subduction into the lower versus upper mantle is consistent with 1) the amount of advective heat transport required out of the lower mantle 2) seismic evidence for a significant fraction of plates stagnating at the transition zone and 3) different spatial patterns of shear wave velocity anomalies across the transition zone that is indicative of decoupling of flow between the upper and lower mantle. Hence, both the geochemical and seimic evidence indicates that the transition zone acts as a partial barrier to mantle flow, providing a simple explanation for having a more processed upper mantle and less processed lower mantle. Melting at mid ocean ridges efficiently samples the upper mantle on timescales of 0.5-1.0 Ga, whereas sampling the lower mantle requires exchange across the transition zone and takes 3-7 times longer.

[1] Allegre et al., *GRL* **23**, 1996.

Theoretical evidence of a mixed adsorption mode of water on Fe₃O₄(001)

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The interaction of water with a mineral surface is a fundamental process towards understanding of the surface reactivity. Based on density functional theory (DFT) calculations we investigate the adsorption of water and its influence on the electronic properties and surface reconstruction of $Fe_3O_4(001)$. Starting from a single water molecule per $(\sqrt{2}x\sqrt{2})R45^\circ$ unit cell, we vary the concentration and configuration of water and hydroxyl groups. The surface phase diagram compiled within the framework of *ab-initio* thermodynamics indicates that a clean *wave-like* distorted bulk termination (modified B-layer) [1] is favorable over a substantial range of O_2 and H_2O partial pressures, but competes with a B-layer with oxygen vacancies in the oxygen poor limit. Such vacancies can promote dissociation of isolated water molecules. With increasing water pressure in the gas phase there is a crossover to a mixed molecular and dissociative adsorption mode. A quantitative low energy electron diffraction (LEED) analysis confirms two distinct Fe-O-distances. DFT and LEED results indicate a suppression of the $(\sqrt{2}x\sqrt{2})R45^\circ$-reconstruction.

[1] R. Pentcheva *et al.*(2005), *Phys. Rev. Lett.* **94**,126101.