

## Hadean isotopic signatures in Mesoarchean pillow basalts, southern West Greenland

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Much debate exists as to the timescales of mantle mixing and the potential longevity in the convecting mantle of early-formed chemical domains. Here we present new evidence, in the form of high precision <sup>142</sup>Nd isotopic compositions from pillow basalts from the 3.075±15 Ga Ivisaartoq greenstone belt, southwest Greenland [1, 2], which demonstrate the persistence of unequivocal Hadean isotopic signatures for >1.5 billion years. Variations in <sup>142</sup>Nd signatures originate in variable Sm/Nd reservoirs formed during the active decay of short half-life and now extinct <sup>146</sup>Sm (T<sub>1/2</sub>=103 Myr). Studies of >3.6 Ga rocks from SW Greenland [3, 4] place the timing of early differentiation resulting in the significant (>10 ppm referenced to modern terrestrial compositions) <sup>142</sup>Nd anomalies in these rocks at >4.45 Ga.

The Ivisaartoq greenstone belt is an association of tholeiitic pillow basalts, ultramafic lavas and rare cherts interpreted to have formed in an intra-oceanic environment now metamorphosed to amphibolite facies. Eighteen samples with MgO ranging from 7.6 wt% in the tholeiites to 26.7wt% in high Mg basalts yield a narrow range of initial ε<sub>143</sub>Nd from +0.8 to +3.2. <sup>142</sup>Nd/<sup>144</sup>Nd measured for five samples show a well resolved, narrow range of positive variations (from +5.5 to +8.5 parts per million) compared with standards and with an external standard reproducibility of ±3 ppm (2σ). Although it is possible to account for these positive <sup>142</sup>Nd signatures by contamination with high <sup>142</sup>Nd Eoarchean materials from tectonically adjacent terranes, this is precluded by <sup>143</sup>Nd, major and trace element mixing relationships. Rather these data provide the youngest (3.0 Ga) evidence for Hadean signatures in the mantle and combined with Eoarchean data [3] directly trace the existence and dilution of Hadean upper mantle domains providing new constraints on mantle dynamics and evolution.

[1] Friend & Nutman (2005) *J. Geol. Soc. Lond.* [2] Polat *et al.* (2009) *Chem. Geol.* [3] Bennett, *et al.* (2007) *Science.* [4] Caro *et al.* (2006) *Geochim. Cosmochim. Acta.*

## First-principles molecular dynamics simulations of hydrous silica glasses and melts

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Over the last decades, amorphous silicates containing several wt.% of water have attracted the interest of many experimental and theoretical research groups due to its important role in magmatic flow in the earth crust [1, 2].

We use *ab initio* molecular dynamics simulations to study a sample of liquid silica containing 3.84 wt.% H<sub>2</sub>O. We find that, for temperatures of 3000 K and 3500 K, water is almost exclusively dissolved as hydroxyl groups and the silica network is partially broken. Water molecules or free O-H groups occur only at the highest temperature but are not stable and disintegrate rapidly. Concerning the diffusion processes, HOSi<sub>2</sub> triclusters and SiO dangling bonds play a decisive role as intermediate states for the hydrogen diffusion [3].

We then quenched these liquid samples to 300 K by employing different quench protocols. We find localized states in the band gap that can be associated to negatively charged Si-O dangling bond which are compensated by positively charged three-fold coordinated oxygens. The positions of these states above the O 2p valence band depends on the local environment of the dangling bonds, in particular on the presence of other defects in their neighborhood, and on the hydrogen bond length [4]. These native defects, which could exist in optical fibers for instance, are compatible with the optical absorption and photoluminescence bands observed in amorphous silica and their dependence in the OH content. If present, these pre-existing defects would play a significant role as precursors in the laser-induced defect formation process.

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