Wet Grain Boundaries of the Earth's Lower Mantle

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The incorporation of water into lower mantle phases has been suggest to influence large scale dynamics of Earth's interior through hydraulic weakening. While much as has been speculated about the various anhydrous and hydrous lower mantle phases, little is known about the partitioning of hydrogen between the crystalline lattice and the surrounding network of grain boundaries. This study establishes partition coefficients for protonic defects between grain boundaries and MgSiO3 Bridgmanite. Exploring pressures of 25-125 GPa and temperatures of 1000-4000K, all formation enthalpies are calculated through plane wave density functional theory as implemented by VASP. Utilising low energy interfaces of MgSiO3 Bridgmanite interfaces as predicted in a recent study (van Driel et al. in prep), it is found that formation enthalpies for hydrogen partitioning can be up 4eV lower than the lattice. Even when considering configuration entropy, it was found that hydrogen preferentially segregates onto the grain boundary. Results show that at grain sizes smaller that 0.1mm, interfaces will act as the dominant sink for protonic defects. However at larger grain sizes, the majority of the total water will be incorporated into the lattice interior. While large grainsizes will result in interfaces no longer acting as the dominant sink, grain boundaries themselves will maintain high concentrations of protonic defects; replacing up to 10% of available magnesium sites. In conjuncture with such high concentrations of protonic defects, a significantly enhancement grain boundary diffusivity is expected.