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Atomistic simulation studies of hydrogen and trace elements in Forsterite

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Olivine [$(MgFe)_2SiO_4$] is a major component of the Earth's upper mantle and a major potential reservoir of H and thus water in the Earth's interior. The mechanisms of water incorporation, as H defects, have been extensively studied because of their influence on the physical properties of forsterite, and on the rheological behavior of the Earth's upper mantle. Water can be incorporated into the crystal structure as H defects associated with either Mg and/or Si vacancies. Previous simulations show that H is most energetically favorable to incorporate into pure forsterite in association with Si vacancies. Trace elements in the mantle may also influence the ability of nominally anhydrous minerals (NAMs) such as olivine to host H and thus influence its distribution in mantle silicates. However, studies dealing with possible H/trace element couples in olivine are much more limited. Computer simulation methods can offer real insights at the atomic level to explore hydrogenand trace elements defects in NAMs.

In this study, we use atomistic simulation methods to investigate relationships between a range of M^{3+} impurity ions (Al, Fe, Ga, Mn, Sc, Lu, Yb, Y, Gd, Eu, Nd and Pu) in combination with H in forsterite, the Mg end member olivine. The aim is to obtain quantitative estimates of the stability of trivalent elements defects in hydrous forsterite at upper mantle pressures and the corresponding substitution mechanisms. Two (M^{3+} H^{+}) incorporation mechanism are investigated; the first with M^{3+}substituting for Si, with an associated OH group and the second with M^{3+} at an Mg site charge balanced by an OH group and a Mg vacancy. The results of our simulations show a strong dependence on the ionic radius of the impurity species and some variation with pressure.. There are also significant structural distortions around the impurity defects. At low pressure (0 GPa), the smaller trivalent cations, (eg. Al, Fe Mn and Ga) substitute into forsterite by replacing Si as: $M^{'}_{Si}$+$OH^{\cdot}_{O3H}$. The larger trivalent cations (eg. Eu, Gd, Lu, Nd, Pu, Y and Yb) however, replace Mg at the M2 site coupled with an Mg1 vacancy as described by $V^{''}_{Mg1} + M^{\cdot}_{Mg2}$+$OH^{\cdot}_{O3H}$. At 12 GPa, the larger impurities (eg. Gd, Eu, Nd and Pu) show a preference for the Mg1 site over Mg2 as $V^{''}_{Mg1} + M^{\cdot}_{Mg1}$+$OH^{\cdot}_{O3H}$. This behaviour is only seen when hydrogen is present. At 12 GPa, all the trace elements enter into the compressed host mineral via the Si vacancy mechanism. The presence of hydrogen could also influence trace element diffusion processes in forsterite, which are closely related to mantle rheology. The incorporation of trace elements coupled with hydrogen could lead to changes in the anisotropic compression of olivine in the mantle and thus is of importance in considering models of mantle rheology.