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Computer modelling of hydrogen defects in spinels

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Two spinels have been investigated, ringwoodite (γ-Mg_2SiO_4) and the germanate spinel (γ-Mg_2GeO_4). Ringwoodite is considered to be the most abundant mineral in the lower part of the transition zone (520-660 km depth) and can incorporate up to 2.7 wt% H_2O in form of OH in its crystal structure [1,2]. This presence of hydrogen can influence its physical and chemical properties and thus the dynamics of the transition zone. As for the germanate spinel, it is stable at atmospheric pressure below 810°C as well as high pressures [3]. A detailed comparison of the physical properties of both spinels with incorporation of hydrogen could tell us about the ability of the germante spinel to be used as an analogue for ringwoodite in experimental studies. We have used atomistic computer simulation techniques to investigate the structures and energies of OH-defects in both spinel phases. We have adopted a breathing shell model within the Mott-Littleton approach as it is implemented in the GULP3.0 code [4].

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Effect of temperature and pressure on water solubility in wadsleyite

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During the last decade, many studies have shown that minerals of the Earth's mantle can contain water-derived species. The minerals from the transition zone (TZ), particularly wadsleyite, can incorporate up to a few weight percent of water [1, 2].

Previous experimental studies indicate that the maximum solubility of water in wadsleyite may vary as a function of pressure and temperature. The aim of this study is to investigate rigorously the potential effect of temperature and pressure on the water solubility of iron-free wadsleyite. Samples were synthesized using a 1000t multi-anvil press at BGI, Bayreuth. One series of experiments were performed at a fixed pressure of 15 GPa and at various temperatures and in a second serie the temperature was fixed at 1200°C and pressure was varied from 13 to 18 GPa. The starting material was a mixture of oxides and hydroxide powders yielding Mg_2SiO_4 + 5wt% H_2O. The water content was quantified by ion microprobe using the Cameca IMS 1270 at CRPG, Nancy.

Results show that at 15 GPa, the water concentration decreases significantly with increasing temperature from 2.5 wt% H_2O at 900°C down to 0.93 wt% H_2O at 1400°C; the corresponding wadsleyite Mg/Si ratios increase from 1.79 to 1.93 over this temperature range. No significant effect of pressure on the water solubility was observed at a constant temperature of 1200°C (~ 2.5 wt% H_2O). The Mg/Si ratio is stable at 1.82 ± 0.02. These results confirm the substitution mechanism proposed by [3] with Mg =2H. Implications for the water-filter transition zone model will be discussed.

This study was supported by the Human Potential Program HPRN-CT-2000-00056 Hydrospec and by DFG.

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