Behavior of hydrogen defects in olivine at high temperature and high pressure: disordering, re-configuration and interaction

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Water in the form of hydrogen defects in olivine strongly influences the physical properties of olivine, thereby being responsible for physical/chemical processes in the deep Earth. Knowledge of hydrogen defects in olivine is fundamental to understand water distribution and its impact on the upper mantle. However, the current explanations of water effects on processes in the deep Earth are mainly based on hydrogen defects observed at ambient conditions. Since hydrogen is highly mobile, the migration of hydrogen between lattice sites at high temperature and high pressure may not be quenchable. Therefore, there arises a question: whether the hydrogen defects in olivine obtained from infrared spectra at ambient conditions are the same as those at the temperature and pressure conditions of the upper mantle? Here, we carry out in situ high-temperature and high-pressure infrared spectroscopic investigations on hydrogen defects in the natural olivine and synthetic Fe-free forsterite. We find that hydrogen defects exhibit disordering at temperature-pressure conditions of the upper mantle, and hydrogen defects corresponding to pure Si vacancies display re-configuration under compression. Interestingly, dehydrogenation experiments of the natural olivine indicate interactions of hydrogen defects. The lost hydrogen of the titanium-clinohumite defects does not completely release out of the crystal. It can migrate to pure Si vacancies and, also, can move to Mg vacancies coupling with trivalent cations. Thus, dehydrogenation and interactions of hydrogen storage sites may be very complex. There may be other reactions among storage sites during dehydrogenation, depending on the chemical compositions, hydrogen storage sites, and the annealing conditions. In conclusion, we report disordering and reconfiguration of hydrogen storage sites at high temperature and high pressure, and also interactions of hydrogen storage sites during dehydrogenation. These are vital for understanding water distribution and processes in the deep Earth.