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Compression mechanisms of the spinel and the perovskite by the first principles calculations

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The structural and elastic properties of materials under high pressure and temperature conditions have been extensively studied both experimentally and theoretically. These kinds of studies have provided us fundamental knowledge on many materials under deep Earth's conditions. Widely accepted models of the Earth assume that Mg2SiO4 based minerals are the major component of the upper mantle, which extends to a depth of 660km. Within the upper mantle, there are three phases, i.e. alpha-olivine, beta-spinel and gamma-spinel phases. Pressure induced phase transitions occur at about 10GPa and 15GPa under low temperature condition from alpha-olivine to beta-spinel phases, and from beta- to gamma-spinels, respectively. Existence of beta-spinel phase leads to the discontinuity in seismic waves velocities at a depth of 410 km. It has been also widely accepted that the dominant mineral phase of the Earth's lower mantle is MgSiO3 perovskite based minerals. Therefore high-pressure behavior of such magnesium-silicates is important for a wide range of geophysical problems, which has been widely studied both experimentally and theoretically.

We performed the first principles calculations for gamma-spinel and MgSiO3 perovskite to investigate change in compression mechanism due to Al and water incorporations into them. Comparison of the bulk parameters for these materials between experiments and our calculations, and mechanisms of Al and water incorporation into gamma-spinel and perovskite are discussed.