SMP46-02 会場:106 時間:5 月 22 日 09:15-09:30

# $MgSiO_3$ ペロブスカイト中のプロトン含有量に及ぼす Al の影響
# Influence of Al incorporation on the amount of protons in $MgSiO_3$ perovskite

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Most of the geoscientists believe that olivine-based minerals form the major constituent in the upper mantle, which extends to a depth of 660 km. Major component of the upper mantle is $Mg_2SiO_4$ in which there are three phases depending upon the depth, i.e., Forsterite (alpha phase) , Wadleyite (beta phase) and Ringwoodite (gamma phase). Pressure induced phase transitions occur at about 10 GPa and 15 GPa under low temperature condition from alpha to beta and from beta to gamma phases, respectively. It is widely accepted that the atmosphere and the oceans of the Earth are formed by degassing of the Earth 's mantle. Most of the water may have been lost or it may still be stored in the Earth 's mantle. If considerable amounts of water are present in the Earth 's mantle, such water plays a key role in the geodynamics of the Earth 's interior, because it affects the melting temperature and the transport properties of minerals as well as their elastic properties. Recent high pressure experiments suggested that main components of the transition zone of the mantle, wadsleyite and ringwoodite, can store significant amount of water [1-4].

On the other hand, some experiments suggested that the pure Mg-perovskite, which is one of the major component of the Earth 's lower mantle, can store tiny amount of water in its structure [5,6]. However, it was reported very recently that $MgSiO_3$ perovskite can store more water when the Al is incorporated [7]. In the present study, the first-principles calculations were carried out to investigate the influence of Al incorporation on the amount of water in $MgSiO_3$ perovskite. Our preliminary results show that the solution energy of protons in $MgSiO_3$ decreases when the Al ions are incorporated.

References

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キーワード: 第一原理計算, 下部マントル, ケイ酸マグネシウムペロブスカイト, 水貯蔵, アルミニウム
Keywords: first-principles calculation, lower mantle, magnesium silicate perovskite, water storage, alminium