Japan Geoscience Union Meeting 2012
(May 20-25 2012 at Makuhari, Chiba, Japan)

SMP48-04 会場:102A 時間:5 月 23 日 14:30-14:45

第一原理計算による含水ケイ酸マグネシウムの圧縮機構の検討
Investigation of compressional mechanism of hydrous magnesium silicate by first-principles calculations

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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], and the lower mantle minerals, consisting of Mg-perovskite, magnesiowustite and Ca-perovskite, can potentially store considerable amounts of water [5]. More recently, the substitution mechanism of protons in wadsleyite was studied experimentally by using neutron diffraction technique [6] and theoretically by the first-principles calculations [7] within the density functional theory (DFT) [8]. However the effects of water solution on their physical properties have not yet been fully understood. Then the first principles DFT calculations are performed here to investigate change in compression mechanism of hydrous Mg_2SiO_4, $MgSiO_3$ and MgO, and influence of proton incorporation on the phase transitions between three polymorphs of Mg_2SiO_4, i.e, forsterite, wadsleyite and ringwoodite, and partitioning of Mg_2SiO_4 into $MgSiO_3$ and MgO. Calculated bulk moduli of hydrous Mg_2SiO_4 have become significantly lower than that of water-free one, in which the calculated result of ringwoodite supports the high pressure experiment [9]. Calculated bulk moduli of hydrous Mg-perovskite and periclase are also much lower (-10%~) than that of anhydrous one. Our free energy calculations suggest that partitioning pressure from hydrous ringwoodite to perovskite and hydrous periclase become significantly larger than that for anhydrous case. If water remains considerable amounts of water in the lower mantle, there has still been possibility that 660 km seismic discontinuity is derived from the partitioning between hydrous minerals.

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キーワード: 第一原理計算, ケイ酸マグネシウム, 相転移, 弾性定数, 体積圧縮率
Keywords: first principles calculation, magnesium silicate, phase transition, elastic modulus, bulk modulus