

Geodynamics Seminar

第324回ジオダイナミクスセミナー

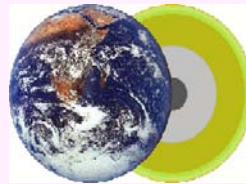
First principles studies on the hydrous wadsleyite and hydrous ringwoodite

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主催: 愛媛大学地球深部ダイナミクス研究センター

日時: 3/23(金) 午後 4時30分～

場所: 総合研究棟 4F 会議室



Abstract

Wadsleyite and ringwoodite are primary constituent minerals in the Earth's transition zone. These phases can contain up to a few wt% H₂O in the crystal structure and are thought to be the most important water reservoirs in the Earth. In recent years, we have investigated the high pressure protonation sites in hydrous wadsleyite using first principles calculation. In this talk, I will review previous studies on hydrous wadsleyite including the structure, elasticity and vibrational properties and introduce our recent attempts on the rheological properties of hydrous wadsleyite by first principles calculation.

There is the most favorable protonation site in wadsleyite crystal structure because of the electric imbalance of this site. On the other hand, the crystal structure of ringwoodite does not have such peculiar protonation site and the reason of such high retention of water in ringwoodite has been unclear so far. In the present study, I have calculated the vibrational properties of hydrous ringwoodite under pressure with various protonation models by first principles. Comparing with the IR and Raman measurements, I will discuss the possible protonation sites in hydrous ringwoodite.

詳細は当センターホームページ: <http://www.ehime-u.ac.jp/~grc/>をご覧ください

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