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High-pressure Raman study of fully deuterated methane hydrate

RYO YABASHI, MASASHI YOSHIDA, TETSUJI KUME, SHIGEO SASAKI, Department of Materials Science and Technology, Gifu University — Methane hydrate (MH: $\text{CH}_4\text{-}n\text{H}_2\text{O}$) crystallizes in a cubic structure I (sI) which consists of hydrogen-bonded water cages which enclathrate methane molecules as guests. With increasing pressure, the initial sI of MH transforms to a hexagonal structure H (sH) at 0.9 GPa, and eventually to an orthorhombic cage-less structure O at 1.9 GPa. The sH consists of three small S1, two small S2, and one large LL water cages in a hexagonal unit cell. The previous high-pressure Raman measurements for C-H stretching vibration of MH-sH indicated that the capacity of methane molecules in the large LL cage abruptly increased at 1.3 GPa, and its occupation number of methane molecule was about 2.5 above 1.3 GPa. However, this result disagrees with the previous high-pressure neutron diffraction experiments for sH of fully deuterated methane hydrate (FDMH: $\text{CD}_4\text{-}n\text{D}_2\text{O}$). To solve this discrepancy, we have carried out the high pressure Raman measurements for C-D stretching vibration in the sI and sH phases of FDMH. As a result, we have obtained the different Raman spectral patterns between FDMH and MH, which suggests that the occupancy of CD_4 in water cages is somewhat different from CH_4 .

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