High pressure study of group-IV clathrate by XRD and Raman scattering

TETSUJI KUME, SHIGEO SASAKI, Gifu University — Group-IV clathrates, which are open-structured Si, Ge, and Sn cage-like compounds, have attracted increasing attention because of their potential applications for thermoelectric devices due to the behavior of phonon-glass and electron-crystal. One of the keys for the intriguing properties is so called rattling vibrations of guests. The direct observation of the rattling is important for understanding of the clathrate properties. Furthermore, the systematic observations of the rattling vibrations as a function of the cage size controlled by pressure are very significant to investigate the guest-host interaction. The pressurization also throws light on the structural stability of the clathrate, which is improved by the guest atoms. The clathrate structure with sp³ network is preserved up to very high pressure. Instead of the structural change, the doped Si clathrates undergo an isostructural phase transition. This paper is concerned with the structural stabilities under high pressure and the rattling vibrations of the guest as a function of the cage size, investigated for various semiconductor clathrates (Sr₈Ga₁₆Ge₃₀, Eu₈Ga₁₆Ge₃₀ and so on) by means of Raman and XRD experiments. On the basis of the recent data, the guest-host interaction is discussed.