Raman spectroscopic investigation of the isotopic effects in graphite

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[Introduction]

Phase Q has higher abundances of heavier noble gases (Ar, Kr, Xe) compared to those in the solar system. Much is already known about the planetary noble gases in Q, but no investigator has ever succeeded to identify this carrier phase itself. Q is only known that it is purely carbonaceous material. Raman spectroscopy in addition to X-ray diffraction study is the useful tools to investigate the graphite material. The typical Raman spectrum of graphite shows G-band (1580cm^{-1}) and D1-band (1350cm^{-1}). The G-band is assigned to the E_{2g} vibration mode of the graphene sheet and is well known. On the other hand, origin of the D1-band in carbon has various opinions (The A_{1g} vibration mode induced by structural defects in the graphene sheet or the coupling between electrons and phonons with the same wave vector near the K-point of the Brillouin zone (Matthews et al.,1999)). We carried out the following research to investigate the isotopic effect and the origin of the D1-band.

[Sample and Experiments]

Sample: ^{12}C amorphous graphite (It is purity 99.9%, and Fe of 3.9ppm is included.), ^{13}C amorphous graphite (It is purity 99.0%, and Fe of 9.7ppm is included.) and Elbogen (Iron meteorite).

Experiments: Raman experiments were performed at Tokyo Medical and Dental University with the spectrometer produced by Kaiser Optical Systems Inc.. An excitation wavelength of 532 nm was used with a YAG-Laser. The laser beam was focused by a microscope with a spot diameter of 2 micrometer.

[Results and Discussions]

Raman spectrum of almost all samples exhibited five bands over the range of 1000 - 3200 cm^{-1}: D1-band (1350cm^{-1}), G-band (1580cm^{-1}), D2-band (1620 cm^{-1}), high frequency doublet G'-band (2700cm^{-1}) and D"-band (2950cm^{-1}). The Raman shift of each bands for ^{13}C amorphous graphite was downshifted from that for ^{12}C amorphous graphite, respectively, and the ratio of these shifts is 0.96. As this value corresponds to the square route of the mass ratio of ^{12}C and ^{13}C, indicating that these Raman bands are due to the lattice vibration mode in diatomic molecule.

We also evaluated the graphite crystallite size (La) by the Knight formula related with the I_{D1}/I_G ratio. Intensity of the D2-band near the G-band was positively correlated with the intensity of the D1-band. Our results suggested that D2-band relate with the distortion of the crystal structure and it is also possible to estimate La in a similar way by using intensity of the D2-band. We rewrote the Knight formula for D2-band.