Nano to micro minerals/materials in Antarctic carbonaceous chondrites

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Various minute minerals are included in matrix of chondrites, especially in carbonaceous chondrite (CC). Carbon minerals, diamond, graphite etc. are such examples (*e.g.*, Lewis et al.,1987; Daulton et al.,1996). Antarctic meteorites may correspond to fall of past meteorite flux different from the present one. Developing mineral extraction method from small meteorite chips is required.

Materials and methods

Ten Antarctic CC (C2,3,5 types) and non-antarctic CC (Murchison, Allende, Orguil and Ivuna) were used. Samples (less than 0.2 ~ 0.3g) were treated by HF, aqua regia, HNO_3, etc.

Results and Discussions

Diamond was found in Antarctic CC; Yamato-86751, Belgica-7904. Murchison and Yamato-86751 contained ball-shaped diamond grains of ~ 30A. It has complicated twin crystal structure. Fullerene-like nano-ball graphite was found and various forms of graphite, such as concentric type, ribbon-like type, etc were also found from Antarctic CC. A "nano ball" shaped graphite had a diameter of 1~ 10 nm and showed good accordance with simulated HRTEM image. Graphite in Murchison is typically in low crystallinity. On the other hand, graphite in Allende has relatively good crystallinity. Antarctic CC were classified into these two types of Muechison and Allende. We discovered another type of carbon rich materials that is fundamentally the same as the materials found from Tagish Lake meteorite (Nakamura, 2002). The material is organic matter with same doughnut-shape structure. This is the second finding of such solid organic matter and the first finding from Antarctic CC (Yamato-793321, Yamato-81020, Yamato-86720, Yamato-86751). This finding implies that the organic matter is included in many CC, in general. So they may be important as materials relating to the early stage processes on the Earth's surface. Characteristic Framboidal magnetite aggregates are found in CI, but .they are not regular (*cf.* Ohfuji & Akai,2002) but irregular type.

References

Daulton et al. (1996),*GCA*,60,4853; Lewis et al. (1987) *Nature* 339, 117; Nakamura et al. (2002) *NIPR Sy. A.,M.* 27,110;Ohfuji & Akai (2002) *Amer Min*.87, 176.

Molecular dynamics simulation of CH_4-CO_2 mixed hydrate

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The molecular dynamics (MD) method was applied to CH_4-CO_2 mixed hydrate (structure I, Pm3n) in order to reproduce and predict the compositional dependence of crystallographic and thermodynamic properties.

The following three types of mixed hydrate crystals were prepared for the simulation:

1) The CH_4 is completely partitioned into S-cage, and CO_2 into M-cage.
2) The CH_4 and CO_2 are evenly distributed to S- and M-cages (Disordered structure).
3) The CO_2 is completely partitioned into S-cage, and CH_4 into M-cage.

The system contains 216 gas molecules (= 54 in S-cage + 162 in M-cage) and 1242 H_2O molecules. The interatomic potential model employed in this study is an empirical one, which can reproduce the dielectric constant, diffusion coefficient, and density for H_2O, the vibration spectrum, density, and structure for CH_4 and CO_2. The MD calculation was carried out under constant temperature and pressure conditions with the step time of 0.4 fs. In each MD run a sufficient long period of aging (more than 100,000 steps) was performed in order to establish steady state of the system. After this, the subsequent period of 50,000 steps was carried out to calculate time-averaged lattice parameter and molar enthalpy.

The characteristic results are as follows:

1) The compositional dependence of lattice parameter

The lattice parameter varies systematically with the CO_2 concentration [= CO_2 / (CH_4 + CO_2)] in M- and S-cages. The lattice parameter of CO_2 hydrate is 0.1 % (100 K, 0.01 GPa) or 0.3 % (300 K, 0.01 GPa) larger than that of methane hydrate. The concentration of CO_2 in S-cage largely affects the lattice parameter.

2) The compositional dependence of molar enthalpy

The structure with the enrichment of CO_2 into M-cage is more stable than the disordered structure, where CH_4 and CO_2 are evenly distributed to both cages. This is consistent with the result of cage occupancy measurements by use of Raman spectroscopy (Nakano and Ohgaki, 2000).