Assessing organic molecules during a deflagration process with quenching effect

Y. Takano[1], K. Yamada[2], C. Okamoto[3], K. Sakamoto[4], T. Sawada[4], R. Okazaki[5], and S. Tachibana[6]

[1]Japan Agency Marine-Earth Science Technology (JAMSTEC), [2]Tokyo Inst. Technology (TIT), [3]Kobe Univ., [4]Japan Aerospace Exploration Agency (JAXA), [5]Kyushu Univ., [6]Hokkaido Univ.
E-mail: takano@jamstec.go.jp

The chemical nature of deflagration and detonation products (*i.e.*, soot) has been investigated mostly into solid materials including formation of amorphous carbon composite and diamond [1]. The physical explosive shock, *i.e.*, a momentary energetic reaction, will also produce simple inorganic gas components (*e.g.*, N_2, CH_4, CO_2, H_2O) as end products. However, the chemical composition for volatile and involatile organic compounds are still largely unknown. To assess those important issues by a physical explosive shock, we conducted a simulation experiment using KTB explosive ($KClO_4$, 69.5%; TiH_2, 19.5%; B, 9.5%; Nitrocellulose, 1.5%) with RK ignition charge explosive ($Pb(SCN)_2$, *ca*. 50%; $KClO_3$, *ca*. 50%; Nitrocellulose, ≤ 1%) under ambient temperature and low pressure (< 40 Pa; Ar-replaced and then vacuumed for substantial time). For the qualitative feedback to projectile operation [2], we also compared the deflagration phenomenon equipped with a sabot and w/o a sabot. After the experiment in the closed box, we collected the gaseous sample, carbonaceous solid samples and relic of burst materials. Here, we discuss the preliminary report on an assessment of organic molecules and inorganic elemental profiles.

Firstly, low molecular weight carboxylic acids, *e.g*., formic acid and acetic acid, were detected by an ion-chromatography (IC) and a thermal desorption-gas chromatography/mass spectrometry (TD-GC/MS [3]). A wide variety of aliphatic hydrocarbons were detected; the series of straight-chain aliphatic hydrocarbons (< n-$C_{20}H_{42}$) were chemically-resemble to the product of putative Fischer-Tropsh Type reaction. Secondly, number of aromatic hydrocarbons and heterocyclic hydrocarbon (*e.g.*, dibenzofurane) were detected; the most abundant species were 1-Ring type of benzene and toluene, which were consistent with the volatile gas analysis by a solid-phase micro-extraction (SPME) coupled with GC/MS. The isomer ratios for 2-methyl and 1-methyl naphthalene (2-MN/1-MN), phenanthrene and anthracene (Phe/Ant) indicated typical signatures of abiotic formation process (cf. detonation process [3]). The relative abundance for those aromatic rings showed 1-Rings > 2-Rings > 3-Rings > 4-Rings. We conclude that the KTB- and RK-based deflagration with the quenching effect will produce various labile and refractory organic matters in the soot without thermal degradation.

[1] *e.g.*, Greiner *et al.*, Diamonds in detonation soot. *Nature* **333**, 440-442 (1988).
[2] Tachibana *et al.*, Hayabusa2: Scientific importance of samples returned from near-Earth C-type asteroid 1999 JU_3. *Geochem. J.*, **48**, 571-587 (2015); Okazaki *et al.*, Hayabusa2 sample container: Metal-seal system for vacuum encapsulation of returned samples. *Space Science Reviews* (submitted)
[3] Takano *et al.*, Abiotic formation of amorphous carbonaceous particles by a HMX (cyclotetramethylenetetranitramine) explosion experiment: implication from organic matters and the quench effect. *Abstract for Hayabusa 2014: 2nd Symposium of Solar System Materials*, P03 (2014)