Two Innovative Devices for DART®-MS Systems

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ionRocket

Direct analysis in real time-mass spectrometry (DART®-MS) enables nearly instantaneous determination of sample composition using mass spectrometry. Therefore, DART-MS is a powerful method for analysis of sample mixtures. However, this method is not suitable for polymer analysis because many polymers are difficult to volatilize.
For polymer analysis by using DART®-MS, we developed an innovative device for DART®-MS, called " ionRocket " (Fig.1, 2), which induces thermal desorption and pyrolysis of samples. The vapor phase of polymer samples was generated by applying a temperature-controlled heating gradient, then ionized and introduced into the mass spectrometer.
In this poster, we describe the analysis applications using the ionRocket combined with DART®-MS.

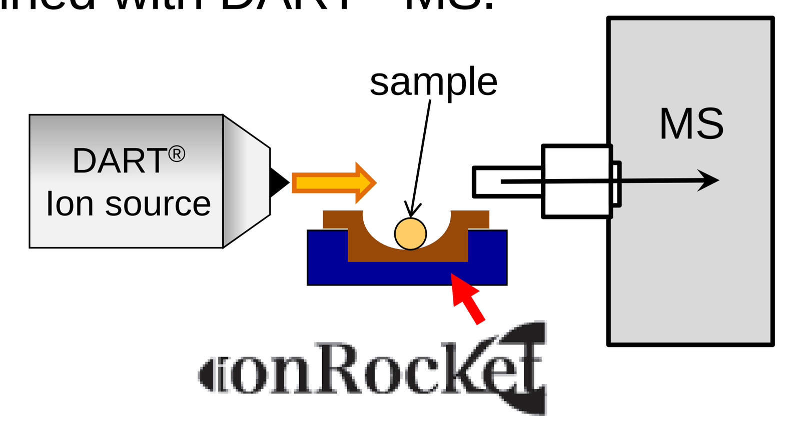


Fig.1 Schematic of ionRocket combined with DART®-MS system

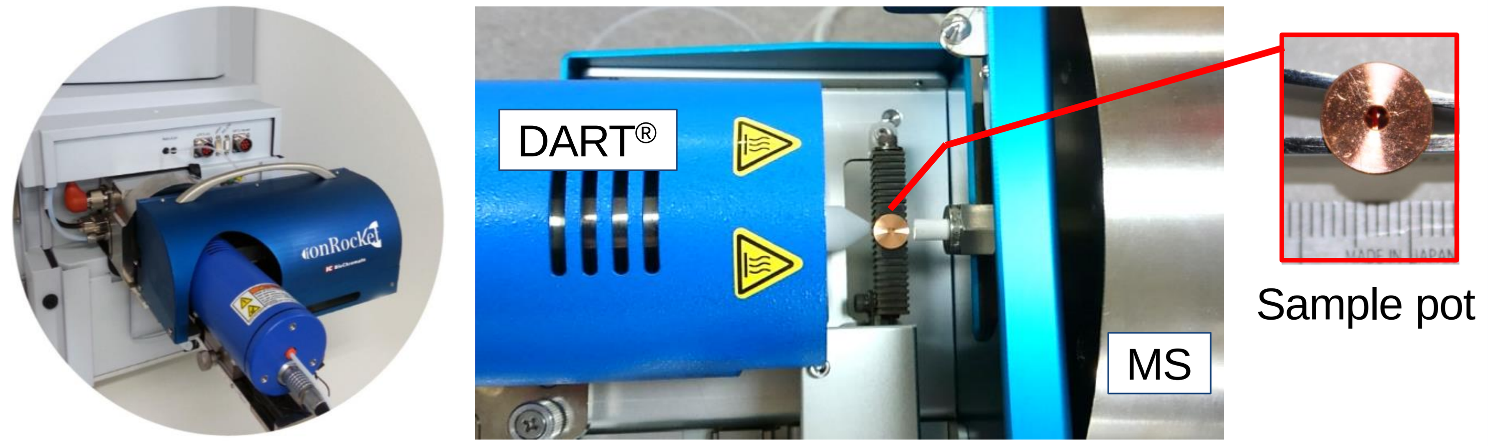


Fig.2 ionRocket combined with DART®-MS system

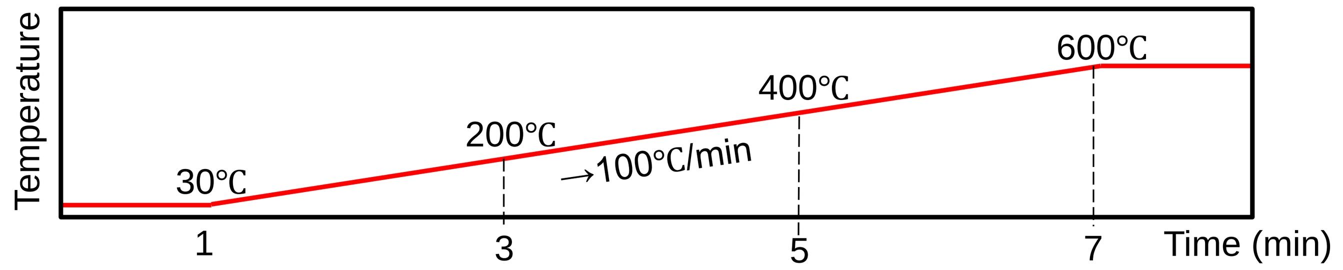
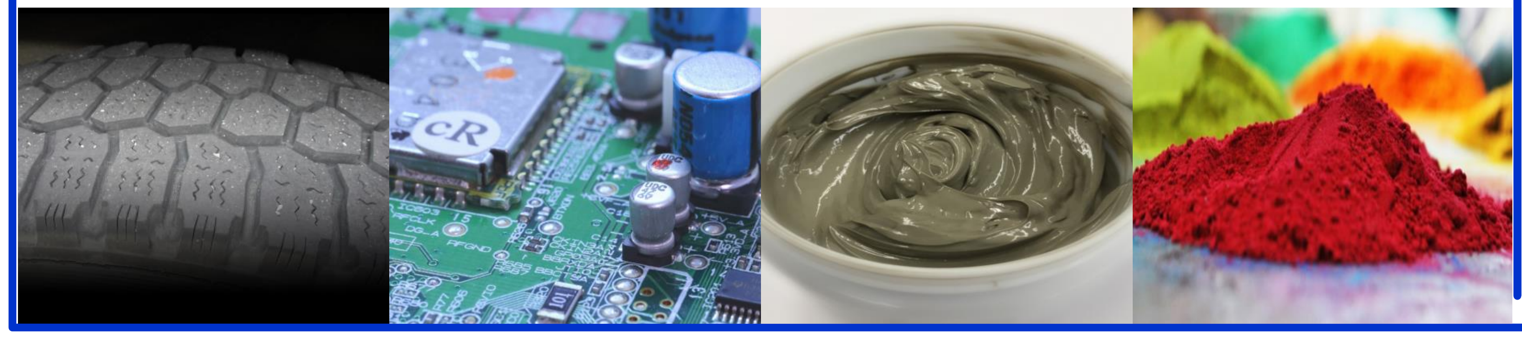
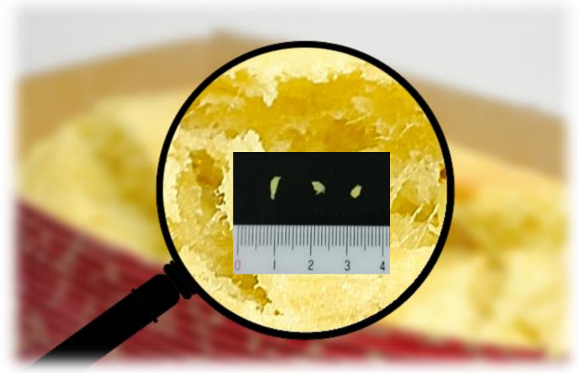


Fig.3 Example of heating condition of ionRocket



Analysis application:
Identification of foreign substances ~PP~

Polypropylene (PP) is various used such as food containers, fibers, household appliances, automobiles, medical parts, etc., and PP is often found as contaminated foreign matter in various manufacturing industries. Although FT-IR is often used as a rapid analysis of foreign matter, it is impossible to identify among the same materials even if it can estimate polymer kinds (Fig.4). ionRocket combined with DART-MS enables identification the foreign substance's where came from by using additive or thermal decomposition pattern as a marker.



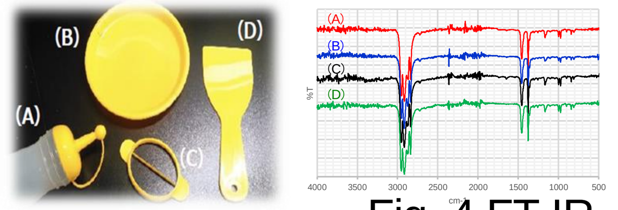


Fig. 4 FT-IR

● Samples

Four kinds of PP products *(A)~(D), manufacturers are different

● Methods

Samples (ca. 0.5 mm x 0.5 mm) were cut and placed into the ionRocket sample pot. A temperature gradient was applied by heating each sample from room temperature to 600 ℃, at a rate of 100 ℃/min (total run time: 7 min.).

● Results

As a results of FT-IR, no significant difference was detected between these samples (Fig. 4).In contrast, samples were identified using the ionRocket combined with DART-MS. Using this method, the total ion chromatogram (TIC) of these samples are shown in Fig. 5. By applying the heat gradient, thermal desorption and pyrolysis reactions were detected. There was a clear distinction between the temperatures at which thermal desorption products were detected. Mass spectra at 200 ℃ (thermal desorption region) were shown in Fig. 6. The additives were different among them. In addition, mass spectra of at 400 ℃ (pyrolysis region) were shown in Fig. 7. Thermal decomposition pattern of PP were detected at this temperature.
It was confirmed that this analysis methods enables identification the foreign substance's where came from by using additive or thermal decomposition pattern as a marker although among the same polymer kinds.
Therefore, this analytical method is useful for R&D and QC.

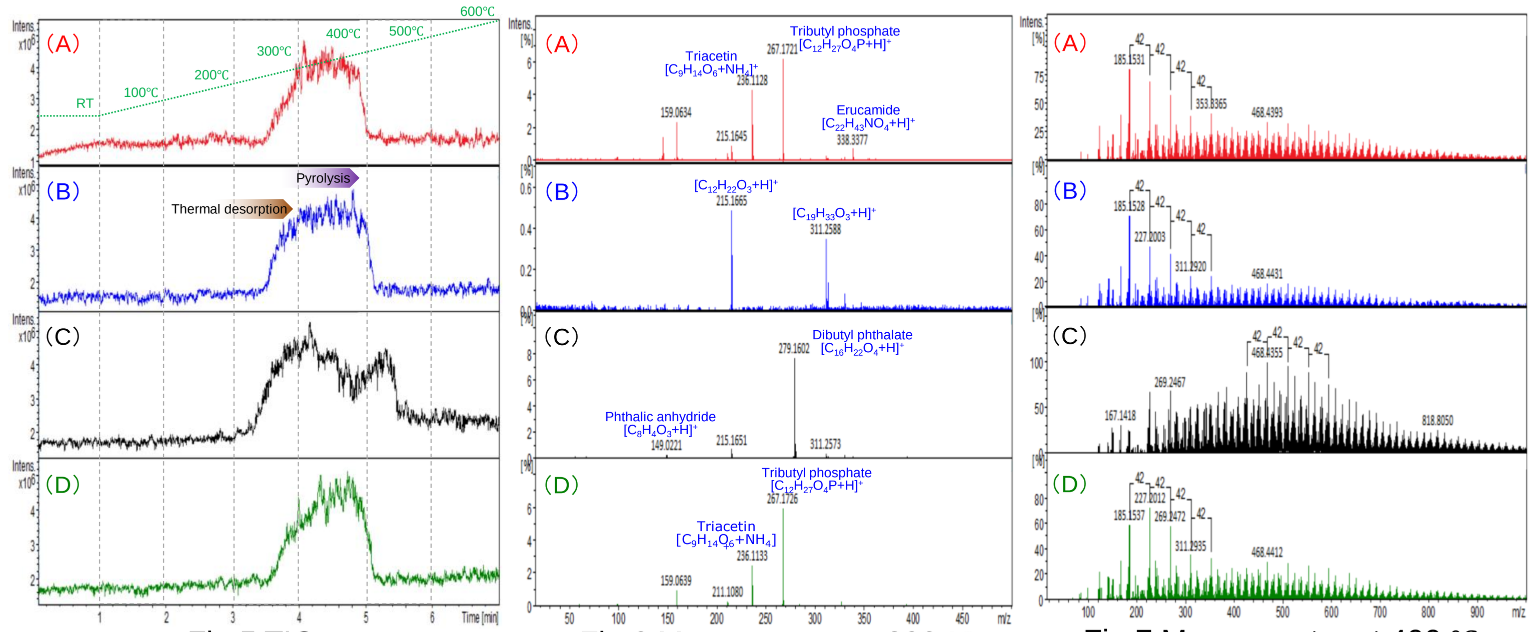


Fig.5 TIC
Fig.6 Mass spectra at 200 ℃
Fig.7 Mass spectra at 400 ℃

Volatimeship

Gas chromatography/mass spectrometry (GC/MS) is typically used for analysis of volatile compounds, such as aromas, flavors, fragrances and outgas. For qualitative analysis, GC/MS is a powerful analysis method, but due to the time required for GC separation, it is not suitable for continuous monitoring like change over time in seconds.
DART®-MS analysis, a direct analysis method, enables near instantaneous determination of sample composition via mass spectrometry. Although DART®-MS also enables determination of volatile compounds, when the samples contain only small amounts of the volatilized target compounds diffusion can make them undetectable in the open environment of the DART®-MS system.
In order to overcome this issue, we developed a closed-chamber interface device called " Volatimeship " (Fig.8). Volatimeship combined with DART®-MS is an effective method to monitor volatile compounds with short analysis times and high sensitivity.

Fig.8 Volatimeship

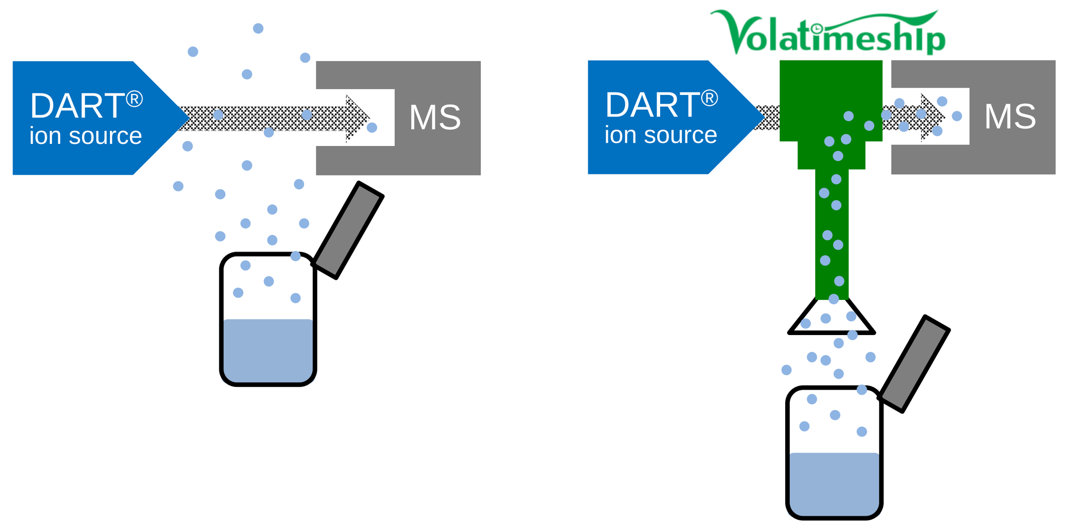


Fig.9 The benefit of Volatimeship

Analysis application:
Realtime Monitoring of Fragrance ~Sake~

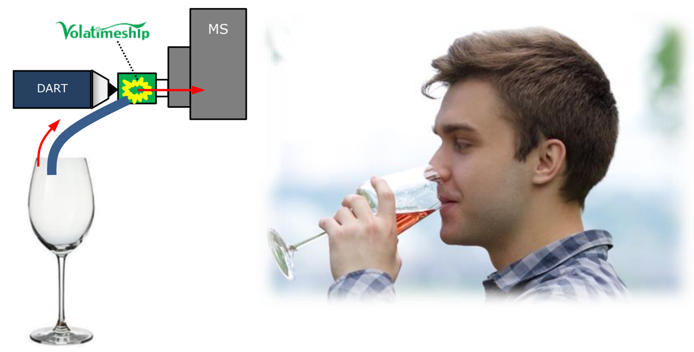
Sake is a Japanese national liquor which is fermented from the raw materials rice, *kome-koji* and water, and many kinds are brewed for different flavor notes, such as fruits, flowers, herbs, and spices. Additionally, sake can be served in a variety of vessels (i.e. cups): the *Choko*, the *Masu*, the *Sakazuki*, or a wineglass, allowing one to enjoy different varieties of scents, depending on the cup. Volatimeship combined with DART-MS enables continuous detection of the change in fragrance intensity directly from the sake vessel.

● Samples

Hakutsuru Daiginjo (i.e., sake)
two cup-types (i.e., *Choko* and wineglass)

● Methods

Sake (30 mL) was added into a cup. Data acquisition via the mass spectrometer were began and the first 30 s measured background. Next, the cup was placed at the introducing tube of the Volatimeship, where the position of the introducing tube approximates the position of human nose where the human are drinking. Then, the volatile compounds were directly detected.



● Results

Ethyl caproate is one of the characteristic fragrances of sake, especially Ginjo and Daiginjyo. As the cup of sake was placed at the introducing tube of the Volatimeship, ethyl caproate was immediately detected by mass spectrometer. The volatilization behavior of ethyl caproate for both cups were measured. The wineglass not only shows sharper increase at the moment of placing the cup, but it also shows better sustainability (Fig.10). As for wineglasses, there were some compound (such as $C_{12}H_{26}O_3$) that were not detected from *Choko* (Fig.11). It means that the fragrance of sake was visualized differently depending on the cup. Moreover, these analysis results support the results of sensory evaluation. Volatimeship combined with DART-MS enables objectively evaluation the sensual sensation of fragrance.

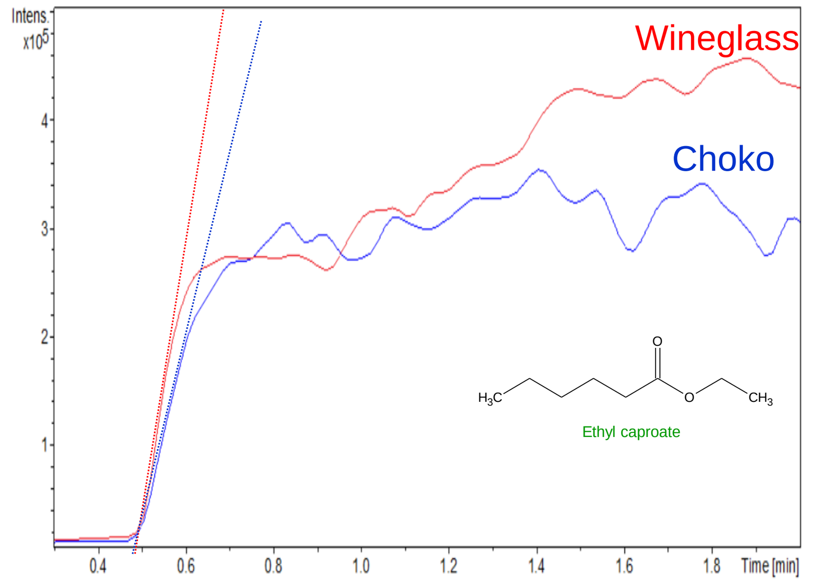


Fig.10 EIC of ethyl caproate

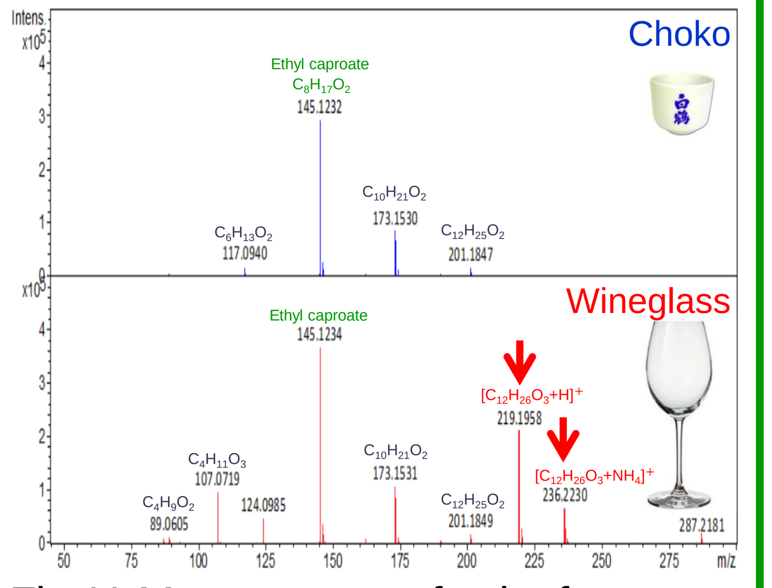


Fig.11 Mass spectra of sake fragrance