

Identifying Surface Contamination using the high throughput MiniSIMS

Mini SIMS



MiniSIMS not only detects superficial organic contaminants but can also discriminate between members of the same polymer family.

- Rapid Analysis of Sub-Monolayer Contamination
- Polymer Identification by Characteristic Peaks
- Determination of Polymer Structure by Library Matching

The cleanliness of a surface is an important property in many industrial situations. In particular, contamination of a substrate surface before paint or other coating material is applied will lead to poor adhesion. Monitoring to detect such contamination is part of the solution, but the full answer requires a precise identification of the contaminant. Complete knowledge about a contaminant indicates the best method for its removal, but more importantly allows its likely source to be traced and eliminated.

When contamination is present as a surface film rather than as a particle, it may be only a monolayer in thickness and invisible to the naked eye. Thin film contamination of this type is frequently organic rather than inorganic in nature, so analysis techniques that only identify the component elements are therefore of limited use. The extra information on molecular structure that is revealed by mass spectrometry is therefore vital in building the complete picture.

It is possible to try to dissolve the contaminant and perform a bulk analysis, but SIMS offers a more convenient and direct method to identify surface contamination in situ. In addition, focusing the primary ion gun gives a spatially resolved analysis that allows the distribution of the contaminant to be established. This distribution may hold additional important clues about the origin of the contamination.

This application note demonstrates how the MiniSIMS provides a fast method to detect and distinguish between similar but different members of the silicone (siloxane) family. The mass spectra show clear and immediate differences as the side chains on a common polymer backbone are varied.

See overleaf for more detailed information.

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The figures show three static SIMS spectra acquired from three contaminated aluminium surfaces. The fast analysis speed of the MiniSIMS allows spectra such as these to be acquired in less than half a minute.

These are the positive SIMS spectra, and in each case there is a corresponding negative SIMS spectrum. For full identification, both spectra would normally be analysed in combination, but for reasons of limited space only the positive spectra are considered here.

The first spectrum (figure 1) is of dimethyl siloxane (PDMS). This is the most widely used silicone, with two methyl groups on each silicon atom in the linear backbone. The elemental peak due to silicon is clearly visible (O is seen in the negative spectrum). The peaks at $m/z = 43$ and $m/z = 73$ are characteristic of the end group of the molecule. The other characteristic peak at $m/z = 147$ represents the first two units in the polymer chain.

The second spectrum (figure 2) is from methyl hydrogen siloxane, where each silicon atom in the chain has one methyl and one hydrogen atom. The tri-methyl end group (represented by the peak at $m/z = 73$) is still the same, but at low mass it can be seen that the molecule fragments differently. The peak at $m/z = 147$ is absent because the relevant structure no longer exists in the parent molecule. At higher mass there are more peaks than was the case for PDMS, because some of the symmetry of the molecule has been lost producing additional fragment ions.

The final spectrum (figure 3) is of methyl glycol siloxane. Here the glycol side chain progressively fragments to give a set of characteristic peaks e.g. between $m/z = 80$ and 120. Again the constant tri-methyl end group is reflected in the peak at $m/z = 73$.

In these examples, the distinctive peaks observed in each spectrum have been explained in terms of individual molecular fragments. This has been done to illustrate why the spectra obtained in the MiniSIMS are representative of very specific members of the same polymer family. However, in routine analysis, it is not necessary to interpret a spectrum to this level of detail. Instead the contaminant spectrum can be compared to library spectra to find the appropriate match.

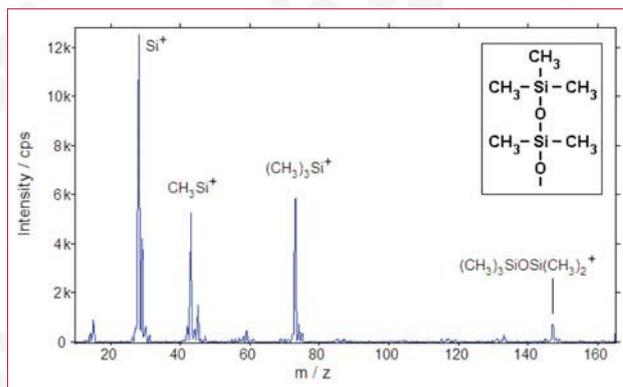


Figure (1) MASS SPECTRUM IDENTIFYING DI-METHYL-SILOXANE

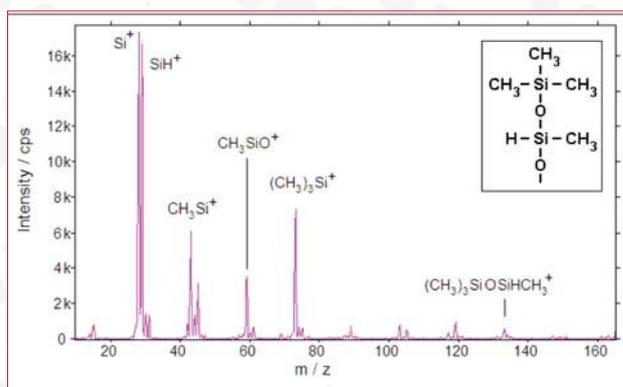


Figure (2) MASS SPECTRUM IDENTIFYING METHYL HYDROGEN-SILOXANE

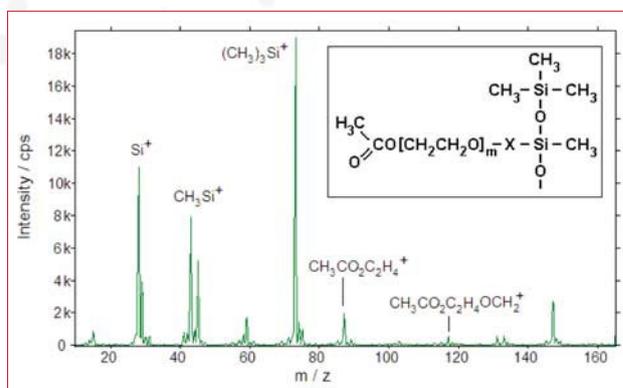


Figure (3) MASS SPECTRUM IDENTIFYING METHYL GLYCOL-SILOXANE