*Journal of Surface Analysis Vol.20, No. 3 (2014) pp. 187−191*
*D. Kobayashi et al. Analysis of TOF-SIMS spectra using quaternary ammonium ions for mass scale calibration*

*Paper*

# Analysis of TOF-SIMS spectra using quaternary ammonium ions for mass scale calibration

Daisuke Kobayashi[*1], Shinya Otomo[2] and Hiroto Itoh[3]
[1]*Research Center, ASAHI GLASS CO., LTD., 1150 Hazawa-cho, Kanagawa-ku, Yokohama, Kanagawa 221-8755 Japan*
[2]*Yokohama R&D Laboratories, Furukawa Electric CO., LTD., 2-4-3 Okano, Nishi-ku, Yokohama 220-0073 Japan*
[3]*Material Analysis Technology Division, KONICAMINOLTA, INC., 1 Sakura-machi, Hino-shi, Tokyo 191-8511 Japan*
*daisuke-kobayashi@agc.com

(Received : November 27, 2013; Accepted : February 11, 2014)

A novel method with quaternary ammonium salts as internal additives has been applied to the mass scale calibration of time-of-flight secondary ion mass spectrometry (TOF-SIMS). Five kinds of quaternary ammonium salts, octyltrimethylammonium bromide (C8TMA), tetradecyltrimethylammonium chloride (C14TMA), octadecytrimethylammonium chloride (C18TMA), cetylpyridinium chloride (CPC) and benzyldimethyltetradecylammonium chloride (Bzl) were diluted with distilled water and conc-$NH_3$ and were mixed in equal quantities. The solution was added to Tinuvin 770 coated on a Si wafer. Then, the sample was measured by TOF-SIMS. The relation between the relative mass accuracy of molecular ions of Tinuvin 770 and the combinations of ions selected for the mass scale calibration was investigated. To improve the mass accuracy of the molecular ion of Tinuvin 770, ions should be selected for the mass scale calibration in the following two ways: one way is for ions to consist only of molecular ions of C8TMA, C14TMA and C18TMA, and the other way is for ions to include the molecular ion of C18TMA, along with the $C_XH_Y$ fragment ions. These results support the proposition of ISO 13084. The novel method with internal additives is effective to improve the mass accuracy of high-mass ions. Quaternary ammonium salts are potential candidates of internal additives.

## 1. Introduction

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) has been recognized as one of the most important surface analysis techniques. TOF-SIMS has features of high mass resolution and wide mass range. To extract information from the TOF-SIMS spectrum, horizontal scale of the spectrum should change from time-of-flight to mass by mass scale calibration. A conventional method for the mass scale calibration is conducted by extrapolation of several identified secondary ions with low mass number [1, 2]. However, identifying an unknown high-mass peak in the spectrum is difficult because an accurate mass scale of the spectrum is not obtained by the conventional method [3]. In 2011, ISO 13084 was formulated in terms of a procedure for the mass scale calibration. According to the ISO 13084, the mass scale calibration should be carried out by the use of some ions with less degradation or fragmentation from the original parent structure. In addition, to identify molecules with a larger mass $m$, the inclusion of an ion with a mass $m_A$ which satisfies $m_A \geq 0.55m$ is highly recommended for the mass scale calibration. The effectiveness of ISO 13084 was confirmed by an interlaboratory study [4]. It is, however, general that TOF-SIMS spectra do not contain correctly identified ions which satisfy $m_A \geq 0.55m$.

A practical method for mass scale calibration in TOF-SIMS has been discussed by the TOF-SIMS working group (TOF-SIMS WG) which was established in Surface Analysis Society of Japan in June 2007 [5 ~ 9]. One of the objectives of TOF-SIMS WG is to figure out a novel mass scale calibration for improvement of the mass accuracy of a high-mass ion. A novel method with quaternary ammonium salts as internal additives has been proposed [9]. ISO 13084 recommendations are met by selection of molecular ions of quaternary ammonium