

Quantification of Li content in organic matrices by Secondary Ion Mass Spectrometry

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The chemical composition of materials has been shown to alter the sputtering and ionization of elements during solid-state secondary ion mass spectrometry (SIMS) measurements, necessitating the use of matrix matched standards to precisely determine elemental abundances. SIMS techniques are being employed frequently on biological and organic samples where matrix compositions are heterogeneous. It is not yet understood how variations of major matrix elements in organic molecules affects the sputtering and ionization of elements from these materials. Carbon glass and single carbon crystals have been used as standards for organic materials, but these materials lack the chemical variability of organic molecules. Therefore, as a first attempt to examine the effect of the major matrix elements of organic molecules on the sputtering and ionization of trace Li in the matrix, we have created ion implant standards in four different organic polymer materials and carbon glass. The matrix compositions consist primarily of C (60-75 wt.%), O (19-33 wt.%) and H (5-8 wt%) which are representative of the bulk chemical compositions of kerogens. We performed SIMS depth profile measurements of Li and C, using both O^- and O_2^- primary ion beams, to determine the Li-content calibration factors, based on Li/C ratios, in the carbonaceous matrices (Table 1). We found no significant trend between the Li calibration factor and the H or O content of the polymer matrices measured using an O_2^- primary ion beam (Figure 1). However, when using an O^- primary ion beam the Li calibration factor is negatively correlated with the O content of the materials with an R^2 value of 0.99. The Li calibration factors were 23-43% smaller (higher Li sensitivity) for all polymers while using O^- instead of O_2^- . Importantly, we found that using a Li ion implant into a glassy carbon matrix provides an acceptable estimation of the Li content in an unknown carbonaceous sample. Thus, our results suggest that while calibration factors derived from measurements using an O_2^- primary beam can be directly used to quantify Li contents in unknown carbonaceous matrices, knowledge of the O content of unknown samples is required, when using the O^- primary beam.

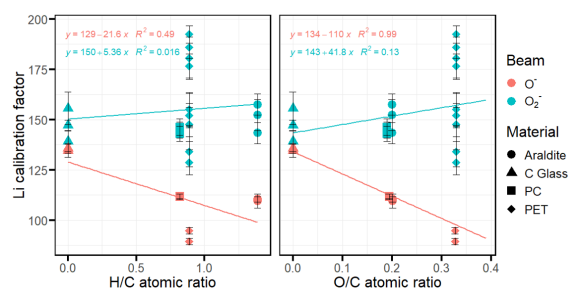


Figure 1. Scatter plots of the Li calibration factors are plotted against the H/C and O/C atomic ratios of polymer and C glass samples for two different primary beams commonly used for measurement of positive Li secondary ions. Li calibration factors of different materials are within error of each other for O_2^- and are correlated with O/C composition while using the O^- primary beam. The $2\sigma_x$ standard errors (S.E.) of individual analyses are plotted.

Table 1. Mean Li calibration factors

| Sample Name | Li calibration factor (O_2^-) | S.E. ($2\sigma_x$) | n | Li calibration factor (O^-) | S.E. ($2\sigma_x$) | n |
|----------------------------------|-----------------------------------|----------------------|----|---------------------------------|----------------------|---|
| Araldite 502 epoxy | 151.0 | 14.4 | 3 | 109.9 | 3.4 | 2 |
| Lexan Polycarbonate (PC) | 144.7 | 5.9 | 3 | 111.7 | 1.5 | 2 |
| Polyethylene terephthalate (PET) | 160.8 | 21.3 | 10 | 92.1 | 7.0 | 2 |
| Carbon Glass | 147.3 | 15.2 | 3 | 135.1 | 4.1 | 2 |

The mean values of Li calibration factors grouped by material and primary beam type are displayed here. The S.E. in this table is the sum of the propagated S.E. errors from the individual analyses and the S.E. for each group in the table above.