# The effect of composition on the local structural environment of Sm and Ta in silicate glasses

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We study the influence of the melt composition on the local structural environment of trace elements in silicate melts. Trace elements are used as petrogenetic indicators of formation processes of igneous rocks, and thus knowledge on their partitioning behaviour during melt crystallization is crucial. This study is motivated by the influence of the melt composition on trace-element partitioning between silicate melt and co-existing crystalline phases as documented in several studies ([1], [2], [3], [4]). The relationship between melt composition and partition coefficients might be understood through the effect of the melt composition on the structural environment of the trace elements as shown by [5] for a few simple melt compositions. Prowatke and Klemme's results [4] from partitioning experiments suggest a significant variation of the structural environment for the lanthanides, Th, Nb and Ta. Therefore, we initiated a study on the elements Sm and Ta in melts of various compositions including those of [4].

Several glasses that vary systematically in composition and nominal polymerization were doped with trace elements (Ta, Sm) at the 500 to 5000 ppm level. Synthesized glass compositions were sodium-trisilicate (NS3) glass, an albite glass and some glass compositions from [4] (ASI200, ASI260).

The spectra were analysed using the software Athena and Artemis by B. Ravel. Amplitudes and phase shift were calculated using Feff and checked on crystalline compounds with known structural parameters ($Ta_2O_5$ and $Sm_2O_3$). So far, only the first coordination shell of Ta and Sm in the glasses was analysed. As it is already evident from the comparison of the Fourier-transforms (Fig. 1), the Ta – O distances obtained for albite and NS3 differ significantly by about 0.5 - 0.7 Å, i.e 1.93±0.02 Å for albite and 1.98 – 2.00 Å for NS3. Sm – O distances vary from 2.31±0.02 Å for NS3 to 2.33±0.02 for ASI200 and 2.35±0.01 for ASI260. Analysis of the Sm spectrum of the albitic composition revealed the presence of a $Sm_2O_3$-like phase, and thus either incomplete equilibration or even Sm saturation of the glass. These differences in the distance to the nearest oxygen neighbours indicate differences in the coordination polyhedron as atomic distances and coordination number are strongly related.

These preliminary observations show that composition-dependant differences in the local structural environment of the studied elements are present and detectable by this method. Such observations would be consistent with previous interpretations by [4], who observed a strong influence of melt composition on trace-element partition coefficients. Those authors explained the influence by a significant change of the structural environment of the trace elements in melts depending on the melt composition. These preliminary results have still to be underpinned by data of better quality that allow also analysis of the second coordination shell. In addition, spectra taken at the K-edge of lanthanides are supposed to improve the insight to coordination environment of these elements.

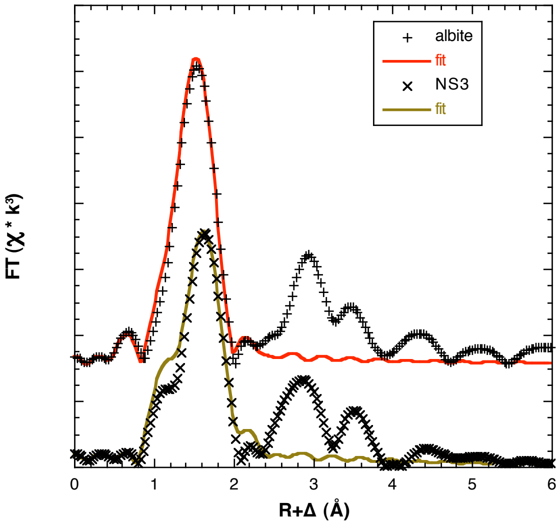

Fig. 1: Fourier-transform of $k^3$-weighted EXAFS and fit of the first shell of Ta in Albite and NS3 glass (5000 ppm Ta).

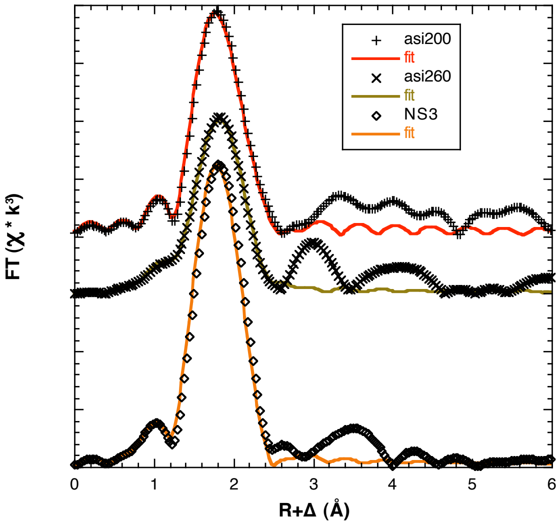

Fig. 2: Fourier-transform of $k^3$-weighted EXAFS and fit of the first shell of Sm in ASI200, ASI260 and NS3 glass (5000 ppm Sm).

# References

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