

Speciation of Fe in silicate glasses and melts by in-situ XANES spectroscopy

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ABSTRACT

In-situ X-ray absorption spectroscopy at the Fe *K*-edge was used to characterize the local structural environment of Fe²⁺ and Fe³⁺ in silicate melts at high temperature (up to 1050 °C) in comparison to their quenched glassy analog at room temperature. Measurements were performed on binary alkali-silicate compositions and on haplogranitic compositions, which were doped with about 5 wt% Fe₂O₃. Changes in the structural environment of Fe were evaluated by analyzing both the pre-edge feature and the first maximum of the EXAFS of the spectra. In most cases, the spectra collected at high temperature differed from those of the quenched samples. At reducing conditions, the melts showed slightly higher amounts of low-coordinated Fe²⁺ than their glassy counterparts. This finding is consistent with results of earlier studies (e.g., Jackson et al. 1993), but the observed change in speciation is smaller than reported by these authors. At oxidizing conditions, glasses and melts displayed a more heterogeneous behavior. The spectra of alkali-silicate compositions indicate higher amounts of low-coordinated Fe³⁺ in the melt, whereas no significant difference between melt and glass was observed for Fe³⁺ in haplogranitic compositions, even if the latter are peralkaline. The amount of non-bridging O atoms in the glass/melt system appears to play an important role particularly for Fe³⁺. However, more complex relationships between Fe and other structural components, especially Al, are possible.

Keywords: XAS (XAFS, XANES), Fe *K*-edge, high-temperature studies, Fe in silicate melts, melt properties, glass properties