European Mineralogical Conference
Vol. 1, EMC2012-481, 2012
European Mineralogical Conference 2012

The influence of melt composition on the local structure around trace elements in glasses and melts with implications for crystal-melt partitioning

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It is generally accepted that the partitioning of trace elements is controlled by temperature, pressure and crystal chemistry (e.g. [1]). However, among others, the results of Prowatke & Klemme [2] on trace element partitioning between melt and titanite, which varied over several orders of magnitude, suggest strong effects of the melt composition on partitioning. Ponader & Brown [3] reported that the coordination of rare earth elements (REE) in quenched melts changes with the degree of polymerization of the melts. However, their data do not allow for a direct correlation between element coordination and partitioning of trace elements.

Here we report melt compositions taken from Prowatke & Klemme [2] that were doped with selected REE (0.5 wt%) and synthesized as glasses. EXAFS was used to constrain the pair distribution function (PDF) of the neighbouring atoms of the REE. Due to the large static disorder around the absorber, the REE – O correlation was described using an asymmetric PDF based on a gamma-like function. The obtained results for the glasses show a increase of the average REE – O distance (e.g. Y – O: 2.27 Å to 2.39 Å ± 0.01 Å; Yb – O: 2.23 Å to 2.37 Å ± 0.01 Å), an increase of coordination number (Y: 6 to 8; Yb: 6 to 7) and a significant increase in the asymmetry of the PDF with increasing alumina saturation index (ASI) of the glass [4]. Furthermore, in-situ high temperature EXAFS on melts were performed to check for possible changes in local structure during quenching. In conclusion, our data show that Y and Yb preferentially bond to non-bridging oxygens in the melt structure, which decrease with increasing ASI. Consequently, over-bonding of bridging oxygens around Y is counterbalanced by an increase of coordination number and Y-O distance to satisfy local charge balance requirements. The adaptations of the trace element coordination to the change in melt composition and structure leads to an increase of the incompatibility of REE in melts.

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