

Structural role of Fe in a pantelleritic melt

Kai-Uwe Hess¹, Nikita Borovkov¹, Thomas Fehr¹, Gabriele Giuli², Corrado Cimarelli¹, Donald B. Dingwell¹

¹Department of Earth and Environmental Sciences, Ludwig Maximilians University, Germany, ²School of Science and Technology, Geology Division, University of Camerino, Italy

E-mail: hess@lmu.de

Iron in silicate melts can play a variety of structural roles involving different coordination numbers and oxidation states. Common Fe species in the melt include 4-Fe²⁺, 5-Fe²⁺, 4-Fe³⁺, and 5-Fe³⁺. The relative proportions between these species can vary considerably according to bulk glass composition and oxygen fugacity conditions. However, in most natural and synthetic silicate glasses 4- and 5- fold coordinated Fe²⁺, and 4-fold coordinated Fe³⁺ are the most common Fe species. Being a major element in silicate melts, Fe can affect considerably important physical properties like density and viscosity of a magma. Moreover, even at constant bulk composition and Fe content, also the Fe oxidation state is known to affect the melt viscosity.

In order to study the Fe structural role in peralkaline silicate melts and its effect on their viscosity, a set of silicate glasses with pantelleritic composition have been synthesized at different oxygen fugacity conditions (ranging from air down to IW buffer). These glasses have been previously characterized by titration to get the Fe oxidation state. Moreover, the viscosity (and glass transition temperature) has been measured for each glass/melt at different temperatures. During the course of this study the glasses were analyzed by ⁵⁷Fe Moessbauer spectroscopy (MB). The spectra were taken at 298K in transmission mode and fitted by applying an extended Voigt-based lineshape according to Botcharnikov et al., 2005. The MB spectra of all samples display three lines which can be described to two different doublets. One doublet with an isomer shift (IS) of ca. 0.9 mm/s relative alpha-iron and a quadrupole splitting (QS) of ca. 2 mm/s can be attributed to ferrous iron. The second doublet with IS of ca. 0.3 mm/s relative alpha-iron and QS of ca. 0.9 mm/s can be attributed to ferric iron. The later values are close to that of ferric iron on tetrahedral site in ferrobaltic glasses (Botcharnikov et al., 2005). With increasing oxidation the QS of ferric iron increases slightly from 0.85 mm/s (0.3 Fe³⁺/Fetotal) to 0.95 mm/s (0.8 Fe³⁺/Fetotal) in contrast to ferrobaltic glasses where a decrease of QS for ferric iron as a function of oxidation was observed. The IS of 0.9 mm/s for ferrous iron remains constant up to an oxidation state of about 0.6 Fe³⁺/Fetotal and with increasing oxidation a rapid decrease to IS of 0.6 mm/s at 0.8 Fe³⁺/Fetotal occurs. At the oxidation state of 0.6 Fe³⁺/Fetotal the constant QS of 2.0 mm/s for ferrous iron increase up to 2.45 mm/s at 0.8 Fe³⁺/Fetotal in contrast to ferrobaltic glasses, where a QS of 2.0 mm/s remains constant over the whole oxidation state (Botcharnikov et al., 2005). In allusion to tektites the doublet with IS of 0.9 mm/s and 0.6 mm/s can be attributed to ferrous iron on a five-fold and four-fold coordinated sites, respectively (Rossano et al., 1999).