

The determination of sulfate and sulfide species in hydrous silicate glasses using Raman spectroscopy

KEVIN KLIMM^{1,*} AND ROMAN E. BOTCHARNIKOV²

¹Institut für Geowissenschaften, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

²Institut für Mineralogie, Leibniz-Universität Hannover, Callinstrasse 3, 30167 Hannover, Germany

ABSTRACT

Raman spectroscopy is used to identify the sulfur speciation (sulfur valence state) in “technical” iron-free soda-lime and potassium-silicate glasses and in “natural” glass compositions such as basalt, andesite, and rhyodacite. The presence of sulfate (S^{6+}) is marked in Raman spectra of oxidized synthetic and natural glasses by bands at ~ 990 and ~ 1000 cm^{-1} , respectively. The presence of sulfide (S^{2-}) in the reduced technical glasses is marked in Raman spectra by a band at 2574 cm^{-1} indicating that S^{2-} is present as HS^- in these Fe-free glasses. Such a band is absent in the Raman spectra of reduced basaltic, andesitic, and rhyodacitic glasses. However, an additional band at ~ 400 cm^{-1} appears in the Raman spectra of the reduced S-bearing “natural” glasses when compared to that of S-free reduced “natural” reference glasses indicating that S^{2-} is most likely complexed with Fe in these glasses. Thus, the dissolution mechanism of S^{2-} appears to be different in Fe-free and Fe-bearing glasses and S^{2-} is dissolved as either HS^- -species or Fe-S complexes, respectively. The data shown here demonstrate the potential of Raman spectroscopy in identifying the sulfur valence state in silicate glasses. In addition, S^{2-} is dissolved as completely different complexes when comparing “technical” iron-free and “natural” iron-bearing, hydrous silicate glass compositions.

Keywords: Raman spectroscopy, silicate glass, sulfur speciation, sulfur valence state