American Mineralogist, Volume 93, pages 235–240, 2008

The origin of S^{4+} detected in silicate glasses by XANES

Max Wilke,[1,*] Pedro J. Jugo,[2,3] Kevin Klimm,[4] Jean Susini,[5] Roman Botcharnikov,[6] Simon C. Kohn,[3] and Markus Janousch[7]

[1]Institut für Geowissenschaften, Universitaet Potsdam, Karl-Liebknecht-Str. 24, 14476 Golm, Germany
[2]Department of Earth Sciences, Laurentian University, 935 Ramsey Lake Road, Sudbury, Ontario P3E 2C6, Canada
[3]Institut für Geowissenschaften, Johann Wolfgang Goethe Universität, Altenhöferalle 1, 60438 Frankfurt, Germany
[4]Department of Earth Sciences, University of Bristol, Wills Memorial Building, Bristol, BS8 1RJ, U.K.
[5]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, BP220, 38043 Grenoble CEDEX, France
[6]Institut für Mineralogie, Leibniz Universitaet Hannover, Callinstr. 3, 30167 Hannover, Germany
[7]Paul Scherrer Institut, Swiss Light Source, 5232 Villigen-PSI, Switzerland

Abstract

The origin of sulfite (S^{4+}) species in silicate glasses was evaluated using XANES at the S *K*-edge. Systematic investigations show that the presence of S^{4+} species in silicate glasses is an analytical artifact related to changes in the sulfur species caused by irradiation with an electron beam during EMPA or by irradiation with an intense focused X-ray beam during synchrotron analysis. The data shown here indicate that S^{2-} and S^{6+} are the only significant sulfur species occurring in silicate glasses synthesized under geologically relevant conditions.

Keywords: XAS (XAFS, XANES), sulfur *K*-edge, glass properties, sulfur oxidation state, beam damage, sulfur speciation